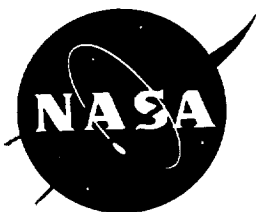


NASA Technical Memorandum 4780
March 1997

110-1
001457
107-11

Microgravity Science & Applications

Program Tasks and Bibliography
for FY 1996



**National Aeronautics and
Space Administration**

Office of Life and Microgravity
Sciences and Applications

Microgravity Science and Applications Division

NASA Technical Memorandum 4780

Microgravity Science & Applications

Program Tasks and Bibliography

For FY1996

*Office of Life and Microgravity Sciences
and Applications*

*Microgravity Science and Applications Division
Code UG
Washington, DC*

National Aeronautics and
Space Administration

Office of Management

Scientific and Technical
Information Program

1997

I. INTRODUCTION	1
II. MICROGRAVITY SCIENCE & APPLICATIONS PROGRAM TASKS	7
 Flight: Biotechnology	
<i>Protein Crystal Growth Vapor-Diffusion Flight Hardware and Facility (Dr. Daniel C. Carter).....</i>	9
<i>Protein Crystal Growth in Microgravity (Dr. Lawrence J. DeLucas).....</i>	11
<i>Electrophoretic Separation of Cells and Particles from Rat Pituitary (Dr. Wesley C. Hymer)</i>	13
<i>Growth, Metabolism, and Differentiation of MIP-101 Carcinoma Cells (Dr. J. M. Jessup)</i>	15
<i>Membrane Transport Phenomena (Mr. Larry W. Mason).....</i>	17
<i>An Observable Protein Crystal Growth Flight Apparatus (Dr. Alexander McPherson, Jr.)</i>	19
<i>Enhanced Dewar Program (Dr. Alexander McPherson, Jr.).....</i>	22
<i>Investigation of Protein Crystal Growth Mechanisms in Microgravity (Dr. Keith B. Ward)</i>	23
 Flight: Combustion Science	
<i>Scientific Support for an Orbiter Middeck Experiment on Solid Surface Combustion (Prof. Robert A. Altenkirch).....</i>	25
<i>Low-Velocity, Opposed-Flow Flame Spread in a Transport-Controlled, Microgravity Environment (Prof. Robert A. Altenkirch)</i>	27
<i>Reflight of the Solid Surface Combustion Experiment with Emphasis on Flame Radiation Near Extinction (Prof. Robert A. Altenkirch).....</i>	29
<i>Gravitational Effects On Laminar, Transitional, and Turbulent Gas-Jet Diffusion Flames (Dr. M. Y. Bahadori)</i>	31
<i>Sooting and Radiation Effects in Droplet Combustion (SEDC) (Prof. Mun Y. Choi).....</i>	34
<i>Candle Flames in Microgravity (Dr. Daniel L. Dietrich).....</i>	38
<i>Investigation of Laminar Jet Diffusion Flames in Microgravity: A Paradigm for Soot Processes in Turbulent Flames (Prof. Gerard M. Faeth).....</i>	40
<i>Unsteady Diffusion Flames: Ignition, Travel, and Burnout (Dr. Frank Fendell).....</i>	44
<i>Fundamental Study of Smoldering Combustion in Microgravity (Prof. A. C. Fernandez-Pello).....</i>	47
<i>Flammability Diagrams of Combustible Materials in Microgravity (Prof. A. C. Fernandez-Pello).....</i>	53
<i>Ignition and the Subsequent Transition to Flame Spread in Microgravity (Dr. Takashi Kashiwagi)</i>	55

<i>The High-Lewis Number Diffusive-Thermal Instability in Premixed Gas Combustion and Low Temperature Hydrocarbon Oxidation and Cool Flames (Dr. Howard G. Pearlman).....</i>	58
<i>Studies of Premixed Laminar and Turbulent Flames at Microgravity (Prof. Paul D. Ronney).....</i>	60
<i>Ignition and Flame Spread of Liquid Fuel Pools (Dr. Howard D. Ross).....</i>	63
<i>Combustion Experiments in Reduced Gravity with Two-Component Miscible Droplets (Prof. Benjamin D. Shaw).....</i>	66
<i>Combustion of Solid Fuel in Very Low Speed Oxygen Streams (Prof. James S. T'ien).....</i>	68
<i>Droplet Combustion Experiment (Prof. Forman A. Williams).....</i>	71

Flight: Fluid Physics

<i>Surface Controlled Phenomena (Prof. Robert E. Apfel).....</i>	75
<i>Two-Phase Gas-Liquid Flows in Microgravity: Experimental and Theoretical Investigation of the Annular Flow (Prof. Vemuri Balakotaiah).....</i>	77
<i>Critical Viscosity of Xenon (Dr. Robert F. Berg).....</i>	79
<i>The Dynamics of Disorder-Order Transitions in Hard Sphere Colloidal Dispersions (Prof. Paul M. Chaikin).....</i>	81
<i>Investigations of Mechanisms Associated with Nucleate Boiling under Microgravity Conditions (Dr. Vijay K. Dhir).....</i>	83
<i>The Melting of Aqueous Foams (Prof. Douglas J. Durian).....</i>	86
<i>Critical Dynamics of Fluids (Prof. Richard A. Ferrell).....</i>	88
<i>Microscale Hydrodynamics Near Moving Contact Lines (Prof. Stephen Garoff).....</i>	90
<i>Geophysical Fluid Flow Cell (Dr. John E. Hart).....</i>	92
<i>Growth and Morphology of Phase Separating Supercritical Fluids (Dr. John Hegseth).....</i>	94
<i>An Experimental Study of Richtmyer-Meshkov Instability in Low Gravity (Dr. Jeffrey W. Jacobs).....</i>	95
<i>Microgravity Segregation in Binary Mixtures of Inelastic Spheres Driven by Velocity Fluctuation Gradients (Prof. James T. Jenkins).....</i>	96
<i>Bubble Dynamics on a Heated Surface (Dr. Mohammad Kassemi).....</i>	99
<i>Interfacial Phenomena in Multilayered Fluid Systems (Prof. Jean N. Koster).....</i>	101
<i>Magnetorheological Fluids: Rheology and Nonequilibrium Pattern Formation (Prof. Jing Liu).....</i>	103
<i>Extensional Rheology Experiment (Prof. Gareth H. McKinley).....</i>	104
<i>Study of Two Phase Gas-Liquid Flow Behavior at Reduced Gravity Conditions (Dr. John McQuillen).....</i>	106
<i>Pool Boiling Experiment (Prof. Herman Merte, Jr.).....</i>	107

<i>Surface Tension-Driven Convection Experiment</i>	
(STDCE-1, STDCE-2) (Prof. Simon Ostrach).....	109
<i>Behavior of Rapidly Sheared Bubbly Suspensions</i> (Prof. Ashok S. Sangani).....	112
<i>Modeling and New Experiment Definition for the VIBES</i> (Prof. Robert L. Sani).....	114
<i>Studies in Electrohydrodynamics</i> (Dr. Dudley A. Saville).....	116
<i>Mechanics of Granular Materials</i> (Dr. Stein Sture).....	117
<i>Thermocapillary Migration and Interactions of Bubbles and</i>	
<i>Drops</i> (Prof. R. S. Subramanian).....	119
<i>Drop Dynamics Investigation</i> (Prof. Taylor G. Wang).....	121
<i>A Study of the Constrained Vapor Bubble Heat Exchanger</i> (Prof. Peter C. Wayner, Jr.).....	123
<i>Physics of Colloids in Space</i> (Prof. David A. Weitz).....	124

Flight: Fundamental Physics

<i>Microgravity Test of Universality and Scaling Predictions Near the Liquid-Gas</i>	
<i>Critical Point of ^3He</i> (Dr. Martin B. Barmatz).....	127
<i>Critical Dynamics in Microgravity</i> (Prof. Robert V. Duncan).....	128
<i>Satellite Test of the Equivalence Principle (STEP)</i> (Prof. C. W. F. Everitt).....	130
<i>Critical Fluid Light Scattering Experiment - ZENO</i> (Prof. Robert W. Gammon).....	132
<i>Confined Helium Experiment (CHeX)</i> (Prof. John A. Lipa).....	134
<i>A New Test of Critical-Point Universality by Measuring the Superfluid Density</i>	
<i>Near the Lambda Line of Helium</i> (Prof. John A. Lipa).....	136

Flight: Materials Science

<i>In Situ Monitoring of Crystal Growth Using MEPHISTO</i> (Dr. Reza Abbaschian).....	137
<i>Coupled Growth in Hypermonotectics</i> (Dr. J. B. Andrews).....	139
<i>Fundamental Aspects of Vapor Deposition and Etching under Diffusion Controlled</i>	
<i>Transport Conditions</i> (Dr. Klaus J. Bachmann).....	142
<i>Investigation of the Relationship between Undercooling and Solidification</i>	
<i>Velocity</i> (Dr. Robert J. Bayuzick).....	144
<i>Experiments on Nucleation in Different Flow Regimes</i> (Dr. Robert J. Bayuzick).....	147
<i>Equiaxed Dendritic Solidification Experiment (EDSE)</i> (Prof. Christoph Beckermann).....	149
<i>Alloy Undercooling Experiments in Microgravity</i>	
<i>Environment</i> (Dr. Merton C. Flemings).....	150
<i>Measurement of the Viscosity and Surface Tension of Undercooled Melts</i>	
<i>Under Microgravity Conditions and Supporting Magnetohydrodynamic</i>	
<i>Calculations</i> (Dr. Merton C. Flemings).....	151
<i>Compound Semiconductor Growth in Low-g Environment</i> (Dr. Archibald L. Fripp).....	153
<i>Gravitational Role in Liquid-Phase Sintering</i> (Prof. Randall M. German).....	155

<i>Isothermal Dendritic Growth Experiment (Prof. Martin E. Glicksman)</i>	159
<i>Physical Properties and Processing of Undercooled Metallic Glass</i>	
<i>Forming Liquids (Dr. William L. Johnson)</i>	163
<i>Thermophysical Properties of Metallic Glasses and Undercooled</i>	
<i>Alloys (Dr. William L. Johnson)</i>	165
<i>Orbital Processing of High Quality Cadmium Telluride (Prof. David J. Larson, Jr.)</i>	167
<i>Orbital Processing of Eutectic Rod-like Arrays (OPERA) (Prof. David J. Larson, Jr.)</i>	169
<i>Crystal Growth of II-VI Semiconducting Alloys by Directional</i>	
<i>Solidification (Dr. Sandor L. Lehoczky)</i>	171
<i>Growth of Solid Solution Single Crystals (Dr. Sandor L. Lehoczky)</i>	173
<i>The Study of Dopant Segregation Behavior During the Growth of GaAs</i>	
<i>in Microgravity (Prof. David H. Matthiesen)</i>	175
<i>GaAs Crystal Growth Experiment (Prof. David H. Matthiesen)</i>	176
<i>Diffusion Processes in Molten Semiconductors (Prof. David H. Matthiesen)</i>	177
<i>Space- and Ground-Based Crystal Growth using Magnetically</i>	
<i>Coupled Baffle (Dr. Aleksandar G. Ostrogorsky)</i>	179
<i>Comparison of Structure and Segregation in Alloys Directionally Solidified in</i>	
<i>Terrestrial and Microgravity Environments (Prof. David R. Poirier)</i>	181
<i>Temperature Dependence of Diffusivities in Liquid Metals (Prof. Franz E. Rosenberger)</i>	183
<i>Self-Diffusion in Liquid Elements (Prof. Franz E. Rosenberger)</i>	185
<i>Particle Engulfment and Pushing by Solidifying Interfaces (Dr. Doru M. Stefanescu)</i>	187
<i>Crystal Growth of ZnSe and Related Ternary Compound Semiconductors by</i>	
<i>Physical Vapor Transport (Dr. Ching-Hua Su)</i>	189
<i>Interface Pattern Selection Criterion for Cellular Structures in Direction</i>	
<i>Solidification (Dr. Rohit K. Trivedi)</i>	191
<i>Coarsening in Solid-Liquid Mixtures (Prof. Peter W. Voorhees)</i>	193
<i>Vapor Growth of Alloy-Type Semiconductor Crystals (Dr. Heribert Wiedemeier)</i>	195

Ground: Biotechnology

<i>The Use of Bioactive Glass Particles as Microcarriers in Microgravity</i>	
<i>Environment (Prof. Portonovo S. Ayyaswamy)</i>	197
<i>Evaluation of Ovarian Tumor Cell Growth and Gene</i>	
<i>Expression (Jeanne L. Becker, Ph.D.)</i>	200
<i>Expansion and Differentiation of Cells in Three-Dimensional Matrices Mimicking</i>	
<i>Physiological Environments (Prof. Rajendra S. Bhatnagar)</i> ..	203
<i>Quantitative, Statistical Methods for Pre-Flight Optimization, and Post-Flight</i>	
<i>Evaluation of Macromolecular Crystal Growth (Dr. Charles W. Carter)</i>	205
<i>Microgravity Simulated Prostate Cell Culture (Prof. Leland W. Chung)</i>	207

<i>Noninvasive Near-Infrared Sensor for Continual Cell Glucose Measurement (Dr. Gerard L. Cote).....</i>	210
<i>A Comprehensive Investigation of Macromolecular Transport During Protein Crystallization (Dr. Lawrence J. DeLucas).....</i>	214
<i>Development of Robotic Techniques for Microgravity Protein Crystal Growth (Dr. Lawrence J. DeLucas).....</i>	216
<i>Macromolecular Crystallization: Physical Principles, Passive Devices, and Optimal Protocols (Dr. George T. DeTitta).....</i>	218
<i>The Effect of Microgravity on the Human Skin Equivalent (Dr. S. D. Dimitrijevic).....</i>	220
<i>Use of Microgravity-Based Bioreactors to Study Intercellular Communication in Airway Cells (Dr. Ellen R. Dirksen).....</i>	223
<i>Microgravity Thresholds for Anti-Cancer Drug Production on Conifer Cells (Dr. Don J. Durzan).....</i>	227
<i>Laser Scattering Tomography for the Study of Defects in Protein Crystals (Dr. Robert S. Feigelson).....</i>	230
<i>Role of Fluid Shear on 3-D Bone Tissue Culture (Prof. John A. Frangos).....</i>	232
<i>Microgravity Studies of Cell-Polymer Cartilage Implants (Lisa E. Freed, M.D., Ph.D.).....</i>	235
<i>Microgravity Tissue Engineering (Lisa E. Freed, M.D., Ph.D.).....</i>	237
<i>Protein and DNA Crystal Lattice Engineering (Dr. D. T. Gallagher).....</i>	243
<i>Microgravity-Based Three-Dimensional Transgenic Cell Models (Steve R. Gonda, Ph.D.).....</i>	244
<i>Lymphocyte Invasion Into Tumor Models Emulated Under Microgravity Conditions In Vitro (Mr. Thomas J. Goodwin, M.S.).....</i>	246
<i>Differentiation of Cultured Normal Human Renal Epithelial Cells in Microgravity (Dr. Timothy G. Hammond).....</i>	249
<i>Excitable Cells and Growth Factors under Microgravity Conditions (Dr. Charles R. Hartzell).....</i>	251
<i>Determining the Conditions Necessary for the Development of Functional Replacement Cartilage Using a Microgravity Reactor (Prof. Carole A. Heath).....</i>	255
<i>The Effects of Microgravity on Viral Replication (John H. Hughes, Ph.D.).....</i>	257
<i>Sensitized Lymphocytes for Tumor Therapy Grown in Microgravity (Dr. Marylou Ingram).....</i>	260
<i>Three-Dimensional Tissue Interactions in Colorectal Cancer Metastasis (Dr. J. M. Jessup).....</i>	263
<i>Use of Rotating Wall Vessel (RWV) to Facilitate Culture of Norwalk Virus (Dr. Philip Johnson, M.D.).....</i>	265

<i>Fibril Formation by Alzheimer's Disease Amyloid in Microgravity (Dr. Daniel A. Kirschner).....</i>	268
<i>Applications of Atomic Force Microscopy to Investigate Mechanisms of Protein Crystal Growth (Dr. John H. Konnert).....</i>	271
<i>Regulation of Skeletal Muscle Development and Differentiation In Vitro by Mechanical and Chemical Factors (Dr. William E. Kraus).....</i>	273
<i>Neuro-endocrine Organoid Assembly in Vitro (Dr. Peter I. Lelkes).....</i>	275
<i>Multidisciplinary Studies of Cells, Tissues, and Mammalian Development in Simulated Microgravity (Prof. Elliot M. Levine).....</i>	278
<i>Analysis of Electrophoretic Transport of Macromolecules using Pulsed Field Gradient NMR (Dr. Bruce R. Locke).....</i>	282
<i>Ground-Based Program for the Physical Analysis of Macromolecular Crystal Growth (Dr. Alexander J. Malkin).....</i>	283
<i>Thyroid Follicle Formation in Microgravity: Three-Dimensional Organoid Construction in a Low-Shear Environment (Andreas Martin, M.D.).....</i>	286
<i>Biological Particle Separation in Low Gravity (Dr. D. J. Morré).....</i>	288
<i>Continuous, Noninvasive Monitoring of Rotating Wall Vessels and Application to the Study of Prostate Cancer (Prof. David W. Murhammer).....</i>	291
<i>Insect-Cell Cultivation in Simulated Microgravity (Prof. Kim O'Connor).....</i>	295
<i>Shear Sensitivities of Human Bone Marrow Cultures (Dr. Bernhard O. Palsson).....</i>	298
<i>Microgravity and Immunosuppression: A Ground-Based Model in the Slow Turning Lateral Vessel Bioreactor (Dr. Neal R. Pellis).....</i>	300
<i>Microgravity Crystallization of Avian Egg White Ovostatin (Dr. Marc L. Pusey).....</i>	302
<i>Isolation of the Flow, Growth and Nucleation Rate, and Microgravity Effects on Protein Crystal Growth (Dr. Marc L. Pusey).....</i>	304
<i>Stem Cell Expansion in Rotating Bioreactors (Dr. Peter J. Quesenberry).....</i>	306
<i>Study of Crystallization and Solution Properties of Redesigned Protein Surfaces (Dr. David C. Richardson).....</i>	308
<i>Convective Flow Effects on Protein Crystal Growth and Diffraction Resolution (Prof. Franz E. Rosenberger).....</i>	310
<i>Nucleation and Convection Effects in Protein Crystal Growth (Prof. Franz E. Rosenberger).....</i>	313
<i>Enhancement of Cell Function in Culture by Controlled Aggregation Under Microgravity Conditions (Prof. W. M. Saltzman).....</i>	316
<i>Robotic Acquisition and Cryogenic Preservation of Single Crystals of Macromolecules for X-Ray Diffraction (Dr. Craig D. Smith).....</i>	319

<i>Influence of Microgravity Conditions on Gene Transfer Into Expanded Populations of Human Hematopoietic Stem Cells (Dr. F. M. Stewart)</i>	321
<i>Mechanisms for Membrane Protein Crystallization: Analysis by Small Angle Neutron Scattering (Dr. David M. Tiede)</i>	323
<i>Preparation and Analysis of RNA Crystals (Dr. Paul Todd)</i>	325
<i>Development of Microflow Biochemical Sensors for Space Biotechnology (Dr. Bruce Towe)</i>	328
<i>Experimental Studies of Protein Crystal Growth Under Simulated Low-Gravity Conditions (Dr. Eugene H. Trinh)</i>	331
<i>Two-Dimensional Protein Crystallization at Interfaces (Dr. Viola Vogel)</i>	333
<i>Automation of Protein Crystallization Experiments: Crystallization by Dynamic Control of Temperature (Dr. Keith B. Ward)</i>	336
<i>Thermal Optimization of Growth and Quality of Protein Crystals (Dr. John M. Wiencek)</i>	337
<i>Search for a Dilute Solution Property to Predict Protein Crystallization (Dr. W. W. Wilson)</i>	339
<i>A Rational Approach for Predicting Protein Crystallization (Dr. W. W. Wilson)</i>	341
<i>Phase Shifting Interferometric Analysis of Protein Crystal Growth Boundaries and Convective Flows (Dr. William K. Witherow)</i>	342
<i>Characterization of Solvation Potentials Between Small Particles (Dr. Charles F. Zukoski)</i>	344

Ground: Combustion Science

<i>Effects of Energy Release on Near Field Flow Structure of Gas Jets (Prof. Ajay K. Agrawal)</i>	346
<i>Radiant Extinction of Gaseous Diffusion Flames (Prof. Arvind Atreya)</i>	348
<i>Multicomponent Droplet Combustion in Microgravity: Soot Formation, Emulsions, Metal-Based Additives, and the Effect of Initial Droplet Diameter (Prof. C. T. Avedisian)</i>	350
<i>Gas-Phase Combustion Synthesis of Metal and Ceramic Nano-Particles (Prof. Richard L. Axelbaum)</i>	352
<i>Development of Advanced Diagnostics for Characterization of Burning Droplets in Microgravity (Dr. William D. Bachalo)</i>	354
<i>Ignition and Combustion of Bulk Metals in Microgravity (Ground-Based Experiment) (Prof. Melvyn C. Branch)</i>	356
<i>Modeling of Microgravity Combustion Experiments - Phase II (Prof. John D. Buckmaster)</i>	358
<i>A Numerical Model for Combustion of Bubbling Thermoplastic Materials in Microgravity (Dr. Kathryn M. Butler)</i>	362

<i>Heterogeneous Combustion of Porous Solid Fuel Particles Under Microgravity: A Comprehensive Theoretical and Experimental Study (Prof. H. K. Chelliah)</i>	364
<i>Buoyancy Effects on the Structure and Stability of Burke-Schumann Diffusion Flames (Prof. L.- D. Chen)</i>	365
<i>Gravitational Effects on Premixed Turbulent Flames: Microgravity Flame Structures (Dr. Robert K. Cheng)</i>	369
<i>Combustion of Interacting Droplet Arrays in a Microgravity Environment (Dr. Daniel L. Dietrich)</i>	370
<i>Internal and Surface Phenomena in Heterogeneous Metal Combustion (Dr. Edward L. Dreizin)</i>	372
<i>Interaction of Burning Metal Particles (Dr. Edward L. Dreizin)</i>	374
<i>Flame-Vortex Interactions Imaged in Microgravity (Prof. James F. Driscoll)</i>	376
<i>Aerodynamic, Unsteady, Kinetic, and Heat Loss Effects on the Dynamics and Structure of Weakly-Burning Flames in Microgravity (Prof. Fokion N. Egolfopoulos)</i>	379
<i>Detailed Studies on the Structure and Dynamics of Reacting Dusty Flows at Normal and Microgravity (Prof. Fokion N. Egolfopoulos)</i>	381
<i>Effects of Gravity on Sheared and Nonsheared Turbulent Nonpremixed Flames (Prof. Said E. Elghobashi)</i>	382
<i>Soot Processes in Freely-Propagating Laminar Premixed Flames (Prof. Gerard M. Faeth)</i>	384
<i>Combustion of Electrostatic Sprays of Liquid Fuels in Laminar and Turbulent Regimes (Prof. Alessandro Gomez)</i>	386
<i>Characteristics of Non-Premixed Turbulent Flames in Microgravity (Dr. Uday Hegde)</i>	389
<i>Three-Dimensional Flow in a Microgravity Diffusion Flame (Prof. Jean R. Hertzberg)</i>	390
<i>Combustion Synthesis of Fullerenes and Fullerenic Nanostructures in Microgravity (Prof. Jack B. Howard)</i>	392
<i>Unsteady Numerical Simulations of the Stability and Dynamics of Flames in Microgravity (Dr. K. Kailasanath)</i>	393
<i>Real Time Quantitative 3-D Imaging of Diffusion Flame Species (Dr. Daniel J. Kane)</i>	395
<i>Soot and Radiation Measurements in Microgravity Turbulent Jet Diffusion Flames (Prof. Jerry C. Ku)</i>	396
<i>Studies of Flame Structure in Microgravity (Prof. Chung K. Law)</i>	398
<i>Chemical Inhibitor Effects on Diffusion Flames in Microgravity (Dr. Gregory T. Linteris)</i>	400
<i>Computational and Experimental Study of Laminar Diffusion Flames in a Microgravity Environment (Prof. Marshall B. Long)</i>	403
<i>Dynamics of Liquid Propellant Combustion at Reduced Gravity (Dr. Stephen B. Margolis)</i>	404
<i>Structure and Dynamics of Diffusion Flames in Microgravity (Prof. Moshe Matalon)</i>	405
<i>Filtration Combustion for Microgravity Applications: (1) Smoldering,</i>	

<i>Filtration Combustion for Microgravity Applications: (1) Smoldering,</i>	
<i>(2) Combustion Synthesis of Advanced Materials (Prof. Bernard J. Matkowsky)</i>	<i>408</i>
<i>Combustion of PTFE: The Effect of Gravity on Ultrafine Particle</i>	
<i>Generation (Prof. J. T. McKinnon)</i>	<i>412</i>
<i>Premixed Turbulent Flame Propagation in Microgravity (Prof. Suresh Menon).....</i>	<i>414</i>
<i>Gravitational Influences on Flame Propagation through Non-Uniform Premixed</i>	
<i>Gas Systems (Dr. Fletcher J. Miller).....</i>	<i>416</i>
<i>A Fundamental Study of the Combustion Syntheses of Ceramic-Metal Composite</i>	
<i>Materials Under Microgravity Conditions - Phase II (Prof. John J. Moore)</i>	<i>418</i>
<i>Stretched Diffusion Flames in Von Karman Swirling Flows (Dr. Vedha Nayagam)</i>	<i>422</i>
<i>Flow and Ambient Atmosphere Effects on Flame Spread at</i>	
<i>Microgravity (Prof. Paul D. Ronney).....</i>	<i>423</i>
<i>Flammability Limits and Flame Dynamics of Spherical Flames in Homogeneous</i>	
<i>and Heterogeneous Mixtures (Prof. Paul D. Ronney).....</i>	<i>425</i>
<i>Combustion Research (Dr. Howard D. Ross)</i>	<i>427</i>
<i>Combustion of Unconfined Droplet Clusters in Microgravity (Dr. Gary A. Ruff)</i>	<i>430</i>
<i>Reduced Gravity Combustion with 2-Component Miscible</i>	
<i>Droplets (Prof. Benjamin D. Shaw).....</i>	<i>432</i>
<i>Quantitative Measurement of Molecular Oxygen in Microgravity</i>	
<i>Combustion (Dr. Joel A. Silver).....</i>	<i>434</i>
<i>Numerical Modeling of Flame-Balls in Fuel-Air Mixtures (Prof. Mitchell D. Smooke)</i>	<i>435</i>
<i>Combustion of Rotating Spherical Premixed and Diffusion Flames in</i>	
<i>Microgravity (Dr. Siavash H. Sohrab).....</i>	<i>437</i>
<i>Diffusion Flame Structure, Shape and Extinction: Geometrical</i>	
<i>Considerations (Prof. Jose L. Torero).....</i>	<i>439</i>
<i>Interactions Between Flames on Parallel Solid Surfaces (Dr. David L. Urban).....</i>	<i>441</i>
<i>Gasless Combustion Synthesis from Elements Under Microgravity: A Study of</i>	
<i>Structure-Formation Processes (Prof. Arvind Varma).....</i>	<i>443</i>
<i>Studies of Wind-Aided Flame Spread Over Thin Cellulosic Fuels in</i>	
<i>Microgravity (Prof. Indrek S. Wichman).....</i>	<i>445</i>
<i>High-Pressure Combustion of Binary Fuel Sprays (Prof. Forman A. Williams)</i>	<i>447</i>
<i>Laser Diagnostics for Fundamental Microgravity Droplet Combustion</i>	
<i>Studies (Dr. Michael Winter).....</i>	<i>449</i>
<i>Combustion of a Polymer (PMMA) Sphere in Microgravity (Dr. Jiann C. Yang)</i>	<i>452</i>

Ground: Fluid Physics

<i>Study of Two-Phase Flow and Heat Transfer in Reduced Gravities</i> (Dr. Davood Abdollahian).....	454
<i>Experimental and Analytical Study of Two-Phase Flow Parameters in Microgravity</i> (Dr. Davood Abdollahian).....	456
<i>Colloids & Nucleation</i> (Prof. Bruce J. Ackerson).....	457
<i>Study of Nonaxisymmetric Liquid Bridges</i> (Prof. J. Iwan D. Alexander).....	459
<i>Stability Limits and Dynamics of Nonaxisymmetric Liquid Bridges</i> (Prof. J. Iwan D. Alexander).....	460
<i>Investigations of Multiple-Layer Convection</i> (Prof. C. D. Andereck).....	462
<i>Electrokinetic Transport of Heterogeneous Particles in Suspensions</i> (Prof. John L. Anderson).....	465
<i>Experimental Study of Liquid Jet Impingement in Microgravity: The Hydraulic Jump</i> (Prof. C. T. Avedisian).....	467
<i>Numerical Simulation of Electrochemical Transport Processes in Microgravity Environments</i> (Prof. Sanjoy Banerjee).....	469
<i>Control of Flowing Liquid Films by Electrostatic Fields in Space</i> (Prof. S. G. Bankoff).....	470
<i>Forced Oscillation of Pendant and Sessile Drops</i> (Dr. Osman A. Basaran).....	472
<i>Studies on the Response of Emulsions to Externally-Imposed Electric and Velocity Fields: Electrohydrodynamic Deformation and Interaction of a Pair of Drops</i> (Dr. James C. Baygents).....	474
<i>Dynamics of Granular Materials</i> (Prof. Robert P. Behringer).....	476
<i>Investigation of Drop Formation by a Vortex Ring in Microgravity</i> (Prof. Luis P. Bernal).....	477
<i>Dynamic Modeling of the Microgravity Flow</i> (Dr. Jeremiah U. Brackbill).....	478
<i>Marangoni Effects in Boiling of Binary Fluid Mixtures Under Microgravity</i> (Prof. Van P. Carey).....	480
<i>Marangoni Instability Induced Convection in Evaporating Liquid Droplets</i> (Dr. An-Ti Chai).....	482
<i>Marangoni Instability Induced Convection in Evaporating Liquid Droplets</i> (Dr. An-Ti Chai).....	484
<i>Rewetting of Monogroove Heat Pipe in Space Station Radiators</i> (Prof. S. H. Chan).....	486
<i>Marangoni and Double-Diffusive Convection in a Fluid Layer Under Microgravity</i> (Prof. Chuan F. Chen).....	488
<i>Transport Phenomena in Stratified Flow in the Presence and Absence of Gravity</i> (Prof. Norman Chigier).....	490

<i>Bubble Dynamics, Two-Phase Flow, and Boiling Heat Transfer in Microgravity</i> (Prof. Jacob N. Chung)	492
<i>Microgravity Particle Dynamics</i> (Dr. Ivan O. Clark).....	493
<i>Structure, Shape Instabilities, and Phase Transitions of Freely Suspended Liquid Crystal Bubbles</i> (Prof. Noel A. Clark).....	497
<i>Structure, Hydrodynamics, and Phase Transitions of Freely Suspended Liquid Crystals</i> (Prof. Noel A. Clark).....	499
<i>Fluid Interface Behavior Under Low- and Zero-Gravity Conditions</i> (Prof. Paul Concus)	501
<i>Fluid Interface Behavior under Low- and Zero-Gravity Conditions</i> (Prof. Paul Concus)	504
<i>Interface Morphology During Crystal Growth: Effects of Anisotropy and Fluid Flow</i> (Dr. Sam R. Coriell).....	505
<i>Phoretic and Radiometric Force Measurements on Microparticles under Microgravity Conditions</i> (Dr. E. J. Davis).....	507
<i>Interaction and Aggregation of Colloidal Biological Particles and Droplets in Electrically-Driven Flows</i> (Prof. Robert H. Davis).....	509
<i>Phase Segregation Due to Simultaneous Migration and Coalescence</i> (Prof. Robert H. Davis).....	511
<i>Cell and Particle Interactions and Aggregation during Electrophoretic Motion</i> (Prof. Robert H. Davis).....	513
<i>Theory of Solidification</i> (Prof. Stephen H. Davis).....	515
<i>Theory of Solidification</i> (Prof. Stephen H. Davis).....	517
<i>Microgravity Foam Structure and Rheology</i> (Prof. Douglas J. Durian).....	518
<i>Magnetothermal Convection in Nonconducting Diamagnetic and Paramagnetic Fluids</i> (Prof. Boyd F. Edwards)	520
<i>Effects of Gravity on Sheared Turbulence Laden with Bubbles or Droplets</i> (Prof. Said E. Elghobashi).....	522
<i>Evaporation, Boiling, and Condensation on/in Capillary Structures of High Heat Flux Two-Phase Devices</i> (Prof. Amir Faghri)	524
<i>The Influence of Gravity on Nucleation, Growth, Stability and Structure in Ordering Soft-Spheres</i> (Prof. Alice P. Gast)	525
<i>The Influence of Gravity on Colloidal Crystallization and Field-Induced Aggregation</i> (Prof. Alice P. Gast).....	527
<i>Material Instabilities in Particulate Systems</i> (Dr. Joe D. Goddard).....	529
<i>Thermoacoustic Effects at a Solid-Fluid Boundary: The Role of a Second-Order Thermal Expansion Coefficient</i> (Dr. Ashok Gopinath).....	530

<i>Fluid Mechanics of Capillary Elastic Instabilities in the Microgravity Environment</i> (Prof. James B. Grotberg).....	531
<i>Capillary-Elastic Instabilities in Microgravity</i> (Prof. James B. Grotberg).....	534
<i>Effects of Convection on the Thermocapillary Motion of Deformable Drops</i> (Prof. Hossein Haj-Hariri).....	536
<i>Instability Mechanisms in Thermally-Driven Interfacial Flows in Liquid-Encapsulated Crystal Growth</i> (Prof. Hossein Haj-Hariri).....	537
<i>Evaporation from a Meniscus within a Capillary Tube in Microgravity</i> (Prof. Kevin P. Hallinan).....	538
<i>A Study of the Microscale Fluid Physics in the near Contact Line Region of an Evaporating Capillary Meniscus</i> (Prof. Kevin P. Hallinan).....	540
<i>Interfacial Transport and Micellar Solubilization Processes</i> (Prof. T. A. Hatton).....	541
<i>Critical Phenomena, Electrodynamics, and Geophysical Flows</i> (Dr. John Hegseth).....	543
<i>A Geophysical Flow Experiment in a Compressible Critical Fluid</i> (Dr. John Hegseth).....	545
<i>Experimental Investigation of Pool Boiling Heat Transfer Enhancement in Microgravity in the Presence of Electric Fields</i> (Dr. Cila Herman).....	546
<i>Nonlinear, Resonance-Controlled Bifurcation Structure of Oscillating Bubbles</i> (Dr. R G. Holt).....	548
<i>Thermocapillary Instabilities and g-Jitter Convection</i> (Prof. George M. Homsy).....	550
<i>Problems in Microgravity Fluid Mechanics: Thermocapillary Instabilities and G-Jitter Convection</i> (Prof. George M. Homsy).....	552
<i>Turbidity of a Binary Mixture Very Close to the Critical Point</i> (Prof. Donald T. Jacobs).....	553
<i>Kinetic and Transport Phenomena in a Microgravity Environment</i> (Prof. David Jasnow).....	554
<i>Surfactant-Based Critical Phenomena in Microgravity</i> (Prof. Eric W. Kaler).....	556
<i>Surfactant-Based Critical Phenomena in Microgravity</i> (Prof. Eric W. Kaler).....	558
<i>Bubble Generation in a Flowing Liquid Medium and Resulting Two-Phase Flow in Microgravity</i> (Dr. Yasuhiro Kamotani).....	559
<i>Instability of Velocity and Temperature Fields in the Vicinity of a Bubble on a Heated Surface</i> (Dr. Mohammad Kassemi).....	560
<i>Stabilization of Thermocapillary Convection by Means of Nonplanar Flow Oscillations</i> (Prof. Robert E. Kelly).....	562
<i>Studies in Thermocapillary Convection of the Marangoni-Bénard Type</i> (Prof. Robert E. Kelly).....	564
<i>Two-Phase Annular Flow in Helical Coil Flow Channels in a Reduced Gravity Environment</i> (Prof. Edward G. Keshock).....	565
<i>Microgravity Heat Transfer Mechanisms in the Nucleate Pool Boiling and Critical Heat Flux Regimes Using a Novel Array of Microscale Heaters</i> (Prof. Junggho Kim).....	567

<i>Investigation of Pool Boiling Heat Transfer Mechanisms in Microgravity using an Array of Surface Mounted Heat Flux Sensors (Prof. Jungho Kim)</i>	568
<i>Molecular Dynamics of Fluid-Solid Systems (Prof. Joel Koplik)</i>	569
<i>Molecular Dynamics of Fluid-Solid Systems (Prof. Joel Koplik)</i>	571
<i>Thermocapillary Convection in Floating Zones under Simulated Reduced Gravity (Prof. Sindo Kou)</i>	573
<i>Thermocapillary Convection in Low Pr Materials under Simulated Reduced-Gravity Conditions (Prof. Sindo Kou)</i>	574
<i>Electric Field Induced Interfacial Instabilities (Dr. Robert E. Kusner)</i>	575
<i>Analysis of Phase Distribution Phenomena in Microgravity Environments (Prof. Richard T. Lahey)</i>	577
<i>The Breakup and Coalescence of Gas Bubbles Driven by the Velocity Gradients of a Non-Uniform Flow (Dr. L. G. Leal)</i>	578
<i>Oscillatory Cross-Flow Electrophoresis: Application to Production Scale Separations (Dr. David T. Leighton)</i>	579
<i>Low Dimensional Models for Thermocapillary Convective Flows in Crystal Growth Processes (Prof. A. Liakopoulos)</i>	581
<i>The Micromechanics of the Moving Contact Line (Prof. Seth Lichter)</i>	583
<i>Absolute and Convective Instability and Splitting of a Liquid Jet at Microgravity (Prof. Sung P. Lin)</i>	584
<i>Absolute and Convective Instability of a Liquid Jet at Microgravity (Prof. Sung P. Lin)</i>	586
<i>Magnetorheological Fluids in Microgravity (Prof. Jing Liu)</i>	588
<i>Rheology of Concentrated Emulsions (Prof. Michael Loewenberg)</i>	590
<i>Investigation of Thermal Stress Convection in Nonisothermal Gases under Microgravity Conditions (Dr. Daniel W. Mackowski)</i>	591
<i>The Dissolution of an Interface Between Miscible Liquids (Prof. James V. Maher)</i>	592
<i>Controlling the Mobility of a Fluid Particle in Space by Using Remobilizing Surfactants (Prof. Charles Maldarelli)</i>	594
<i>Stabilization and Low Frequency Oscillations of Capillary Bridges with Modulated Acoustic Radiation Pressure (Prof. Philip L. Marston)</i>	597
<i>Passive or Active Radiation Stress Stabilization of (and Coupling to) Liquid Bridges and Bridge Networks (Prof. Philip L. Marston)</i>	599
<i>Study of Disturbances in Fluid-Fluid Flows in Open and Closed Systems (Prof. Mark J. McCready)</i>	600
<i>Fundamental Processes of Atomization in Fluid-Fluid Flows (Prof. Mark J. McCready)</i>	602
<i>Study of Forced Convection Nucleate Boiling in Microgravity (Prof. Herman Merte, Jr.)</i>	603
<i>A Study of Nucleate Boiling with Forced Convection in Microgravity (Prof. Herman Merte, Jr.)</i>	605

<i>Determination of Interfacial Rheological Properties through Microgravity Oscillations of Bubbles and Drops (Dr. Ali Nadim).....</i>	606
<i>NMRI Measurements and Granular Dynamics Simulations of Segregation of Granular Mixtures (Prof. Masami Nakagawa).....</i>	608
<i>Control of Oscillatory Thermocapillary Convection in Microgravity (Prof. G. P. Neitzel).....</i>	610
<i>Non-Coalescence Effects in Microgravity (Prof. G. P. Neitzel).....</i>	612
<i>Production of Gas Bubbles in Reduced Gravity Environments (Dr. Hasan N. Oguz).....</i>	613
<i>Waves in Radial Gravity using Magnetic Fluid (Dr. Daniel R. Ohlsen).....</i>	615
<i>Industrial Processes (Prof. Simon Ostrach).....</i>	616
<i>Industrial Processes Influenced by Gravity (Prof. Simon Ostrach).....</i>	618
<i>Marangoni Effects on the Bubble Dynamics in a Pressure Driven Flow (Prof. Chang-Won Park).....</i>	620
<i>Nonlinear Dynamics and Nucleation Kinetics in Near-Critical Liquids (Prof. Alexander Z. Patashinski).....</i>	621
<i>Two-Phase Interfaces in Weak External Fields (Prof. Jerome K. Percus).....</i>	623
<i>On the Boundary Conditions at an Oscillating Contact Line: A Physical/Numerical Experimental Program (Dr. Marc Perlin).....</i>	624
<i>Fluid Dynamics and Solidification of Molten Solder Droplets Impacting on a Substrate in Microgravity (Dr. Dimos Poulikakos).....</i>	626
<i>Acoustic Bubble Removal from Boiling Surfaces (Prof. Andrea Prosperetti).....</i>	627
<i>Containerless Ripple Turbulence (Dr. Seth J. Putterman).....</i>	628
<i>Decoupling the Role of Inertia and Gravity on Particle Dispersion (Dr. Chris B. Rogers).....</i>	629
<i>Studies of Radiation-Driven and Buoyancy-Driven Fluid Flows and Transport (Prof. Paul D. Ronney).....</i>	631
<i>Fluid Creep Effects on Near-Wall Solute Transport for Non-Isothermal Ampoules and Suspended Particle Transport Coefficients (Prof. Daniel E. Rosner).....</i>	633
<i>Design/Interpretation of Microgravity Experiments to Obtain Fluid/Solid Boundary Conditions in Non-Isothermal Systems (Prof. Daniel E. Rosner).....</i>	635
<i>Gas Flow from Porous Media and Microgravity Battery Spills (Dr. Robert T. Ruggeri).....</i>	636
<i>Ground Based Studies of Thermocapillary Flows in Levitated Drop (Prof. Satwindar S. Sadhal).....</i>	637
<i>Ground Based Studies of Internal Flows in Levitated Laser-Heated Drops (Prof. Satwindar S. Sadhal).....</i>	640
<i>Effects of Gravity and Shear on the Dynamics and Stability of Particulate and Multiphase Flows (Prof. Ashok S. Sangani).....</i>	641
<i>Dielectric and Electrohydrodynamic Properties of Suspensions (Dr. Dudley A. Saville).....</i>	643

<i>Terrestrial Experiments on G-Jitter Effects on Transport and Pattern Formation</i> (Dr. Michael F. Schatz).....	645
<i>Free-Surface and Contact-Line Motion of Liquids in a Microgravity Environment</i> (Dr. Leonard W. Schwartz).....	646
<i>Drop Breakup in Flow through Fixed Beds as Model Stochastic Strong Flows</i> (Dr. Eric S. Shaqfeh).....	648
<i>Electrohydrodynamic Pool Boiling in Reduced Gravity</i> (Prof. Benjamin D. Shaw).....	650
<i>Transport Processes Research</i> (Dr. Bhim S. Singh).....	652
<i>Solute Nucleation and Growth in Supercritical Fluid Mixtures</i> (Dr. Gregory T. Smedley).....	655
<i>Behavior of Unsteady Thermocapillary Flows</i> (Prof. Marc K. Smith).....	657
<i>The Development of Novel, High-Flux, Heat Transfer Cells for Thermal Control in Microgravity</i> (Prof. Marc K. Smith).....	659
<i>Dynamics of the Molten Contact Line</i> (Dr. Ain A. Sonin).....	660
<i>Marangoni Effects on Drop Deformation and Break-Up in an Extensional Flow: The Role of Surfactant Physical Chemistry</i> (Dr. Kathleen J. Stebe).....	662
<i>Flow-Influenced Shape Stability: Breakup in Low Gravity</i> (Prof. Paul H. Steen)	663
<i>Stability of Shapes Held by Surface Tension and Subjected to Flow</i> (Prof. Paul H. Steen).....	665
<i>Interactions of Bubbles and Drops in a Temperature Gradient</i> (Prof. R. S. Subramanian).....	667
<i>Instability in Surface-Tension-Driven Benard Convection</i> (Prof. Harry L. Swinney)	668
<i>Instabilities in Surface-Tension-Driven Convection</i> (Prof. Harry L. Swinney).....	670
<i>Crystal Growth and Fluid Mechanics Problems in Directional Solidification</i> (Prof. Saleh Tanveer)	672
<i>Crystal Growth and Fluid Mechanics Problems in Directional Solidification</i> (Prof. Saleh Tanveer).....	674
<i>Microgravity Effects on Transendothelial Transport</i> (Dr. John M. Tarbell)	677
<i>Oscillatory/Chaotic Thermocapillary Flow Induced by Radiant Heating</i> (Dr. Robert L. Thompson).....	679
<i>Light Scattering Studies of Relative Motions of Solid Particles in Turbulent Flows</i> (Prof. Penger Tong).....	680
<i>Studies of Particle Sedimentation by Novel Scattering Techniques</i> (Prof. Penger Tong)	682
<i>Acoustic Streaming in Microgravity: Flow Stability and Heat Transfer Enhancement</i> (Dr. Eugene H. Trinh)	684
<i>Computational Studies of Drop Collision and Coalescence</i> (Prof. Grétar Tryggvason).....	686
<i>Nonlinear Bubble Interactions in Acoustic Pressure Fields</i> (Prof. John Tsamopoulos).....	688
<i>Residual Accelerations in a Microgravity Environment</i> (Prof. Jorge Viñals).....	691
<i>Fluid Physics in a Stochastic Acceleration Environment</i> (Prof. Jorge Viñals).....	693
<i>Experimental Study of the Vapor Bubble Thermosyphon</i> (Prof. Peter C. Wayner, Jr.).....	695

<i>Study of Two Phase Flow Dynamics and Heat Transfer at Reduced Gravity</i> (Prof. Larry Witte).....	697
<i>Interactions Between Solidification and Compositional Convection in Alloys</i> (Prof. M. G. Worster).....	699
<i>Nucleation and Chiral Symmetry Breaking under Hydrodynamic Flows</i> (Dr. Xiao-lun Wu).....	701
<i>Oscillatory Thermocapillary Convection</i> (Prof. Abdelfattah Zebib).....	704

Ground: Fundamental Physics

<i>Superfluid Transition of ^4He in the Presence of a Heat Current</i> (Prof. Guenter Ahlers).....	706
<i>The Superfluid Transition of ^4He Under Unusual Conditions</i> (Prof. Guenter Ahlers).....	708
<i>Microgravity Test of Universality and Scaling Predictions Near the Liquid-Gas Critical Point of ^3He</i> (Dr. Martin B. Barmatz).....	710
<i>New Phenomena in Strongly Counterflowing He-II near Tl</i> (Dr. Stephen T. Boyd).....	712
<i>Prediction of Macroscopic Properties of Liquid Helium from Computer Simulation</i> (Prof. David M. Ceperley).....	713
<i>Measurement of the Heat Capacity of Superfluid Helium in a Persistent-Current State</i> (Dr. Talso C. Chui).....	714
<i>Nonequilibrium Phenomena Near the Lambda Transition of ^4He</i> (Dr. Talso C. Chui).....	715
<i>The Lambda Transition Under Superfluid Flow Conditions</i> (Dr. Talso C. Chui).....	716
<i>Nucleation of Quantized Vortices from Rotating Superfluid Drops</i> (Prof. Russell J. Donnelly).....	717
<i>Nucleation of Quantized Vortices from Rotating Superfluid Drops</i> (Prof. Russell J. Donnelly).....	718
<i>Kinetic and Thermodynamic Studies of Melting-Freezing of Helium in Microgravity</i> (Prof. Charles Elbaum).....	719
<i>Kinetic and Thermodynamic Studies of Melting-Freezing of Helium in Microgravity</i> (Prof. Charles Elbaum).....	721
<i>Critical Dynamics of Ambient Temperature and Low Temperature Phase Transitions</i> (Prof. Richard A. Ferrell).....	723
<i>Dynamics of Superfluid Helium in Low Gravity</i> (Mr. David J. Frank).....	726
<i>Investigation of Future Microgravity Atomic Clocks</i> (Prof. Kurt Gibble).....	728
<i>Condensate Fraction in Superfluid Helium Droplets</i> (Prof. J. Woods Halley).....	729
<i>Ultra-Precise Measurements with Trapped Atoms in a Microgravity Environment</i> (Dr. Daniel J. Heinzen).....	732
<i>Precision Measurements with Trapped, Laser-Cooled Atoms in a Microgravity Environment</i> (Dr. Daniel J. Heinzen).....	734
<i>Collisional Frequency Shifts near Zero-Energy Resonance</i> (Prof. Randall G. Hulet).....	736

<i>Dynamic Measurement Near the Lambda-Point in a Low-g Simulator on the Ground (Dr. Ulf E. Israelsson)</i>	737
<i>Dynamic Measurements along the Lambda Line of Helium in a Low-Gravity Simulator on the Ground (Dr. Ulf E. Israelsson)</i>	739
<i>Atom Interferometry in a Microgravity Environment (Dr. Mark A. Kasevich)</i>	741
<i>Static Properties of ^4He in the Presence of a Heat Current in a Low-Gravity Simulator (Dr. Melora E. Larson)</i>	744
<i>Second Sound Measurements near the Tricritical Point in ^3He - ^4He Mixtures (Dr. Melora E. Larson)</i>	745
<i>Effect of Confinement on Transport Properties by Making use of Helium Near the Lambda Point (Prof. John A. Lipa)</i>	746
<i>Red-Shift Test of General Relativity on Space Station Using Superconducting Cavity Oscillators (Prof. John A. Lipa)</i>	747
<i>A Renewal Proposal to Study the Effect of Confinement on Transport Properties by Making Use of Helium along the Lambda Line (Prof. John A. Lipa)</i>	748
<i>Theoretical Studies of the Lambda Transition of Liquid ^4He (Prof. Efstratios Manousakis)</i>	749
<i>Theoretical Studies of Liquid ^4He near the Superfluid Transition (Prof. Efstratios Manousakis)</i>	751
<i>Dynamics and Morphology of Superfluid Helium Drops in a Microgravity Environment (Prof. Humphrey J. Maris)</i>	753
<i>Equilibration in Density and Temperature Near the Liquid-Vapor Critical Point (Prof. Horst Meyer)</i>	755
<i>Density Equilibration in Fluids near the Liquid-Vapor Critical Point (Prof. Horst Meyer)</i>	757
<i>Indium Mono-ion Oscillator II (Prof. Warren Nagourney)</i>	759
<i>Nonlinear Relaxation and Fluctuations in a Non-Equilibrium, Near-Critical Liquid with a Temperature Gradient (Prof. Alexander Z. Patashinski)</i>	760
<i>Superfluid Density of Confined ^4He near Tl (Dr. David Pearson)</i>	762
<i>Finite Size Effects near the Liquid-Gas Critical Point of ^3He (Dr. Joseph Rudnick)</i>	763
<i>Dynamics and Morphology of Superfluid Helium Drops in a Microgravity Environment (Prof. George M. Seidel)</i>	765
<i>Precise Measurements of the Density and Thermal Expansion of ^4He Near the Lambda Transition (Dr. Donald M. Strayer)</i>	766
<i>Precise Measurements of the Density and Critical Phenomena of Helium near Phase Transitions (Dr. Donald M. Strayer)</i>	768

Ground: Materials Science

<i>Analysis of Residual Acceleration Effects on Transport and Segregation During Directional Solidification of Tin-Bismuth in the MEPHISTO Furnace Facility (Prof. J. Iwan D. Alexander)</i>	770
<i>Synthesis and Characterization of Single Macromolecules: Mechanistic Studies of Crystallization and Aggregation (Dr. Spiro D. Alexandratos)</i>	772
<i>Microgravity Impregnation of Fiber Preforms (Dr. M. C. Altan)</i>	774
<i>An Electrochemical Method to Visualize Flow and Measure Diffusivity in Liquid Metals (Dr. Timothy J. Anderson)</i>	777
<i>A Novel Electrochemical Method for Flow Visualization (Dr. Timothy J. Anderson)</i>	778
<i>The Effects of Convection on Morphological Stability during Coupled Growth in Immiscible Systems (Dr. J. B. Andrews)</i>	780
<i>Foam Metallic Glasses (Prof. Robert E. Apfel)</i>	782
<i>Ostwald Ripening of Liquid and Solid Droplets in Liquid Metal Matrices (Dr. Alan J. Ardell)</i>	784
<i>Nucleation and Cluster Formation in Levitated Droplets (Prof. Stephen Arnold)</i>	786
<i>Molecularly Tailored Surfaces via Self-Assembly Processes: Synthesis, Characterization and Modeling (Dr. Mark A. Barteau)</i>	788
<i>Studies of Nucleation and Growth of Intermetallic Compounds (Dr. Robert J. Bayuzick)</i>	790
<i>Transport Phenomena During Equiaxed Solidification of Alloys (Prof. Christoph Beckermann)</i>	793
<i>Equiaxed Dendritic Solidification Experiment (Prof. Christoph Beckermann)</i>	795
<i>Gravitational Effects on the Development of Weld-Pool and Solidification Microstructures in Metal Alloy Single Crystals (Dr. Lynn A. Boatner)</i>	797
<i>Dispersion Microstructure and Rheology in Ceramics Processing (Dr. John F. Brady)</i>	799
<i>Combustion Synthesis of Materials in Microgravity (Dr. Kenneth Brezinsky)</i>	800
<i>Modeling of Convection and Crystal Growth in Directional Solidification of Semiconductor and Oxide Crystals (Dr. Robert A. Brown)</i>	802
<i>Microstructure Formation During Directional Solidification of Binary Alloys Without Convection: Experiment and Computation (Dr. Robert A. Brown)</i>	804
<i>Application of Parallel Computing for Two- and Three-Dimensional Modeling of Bulk Crystal Growth and Microstructure Formation (Dr. Robert A. Brown)</i>	806
<i>Evolution of Crystal and Amorphous Phase Structure During Processing of Thermoplastic Polymers (Prof. Peggy Cebe)</i>	808
<i>Optical Properties for High Temperature Materials Research (Dr. Ared Cezairliyan)</i>	810
<i>Thermophysical Properties of High Temperature Liquid Metals and Alloys (Dr. Ared Cezairliyan)</i>	812

<i>Three-Dimensional Velocity Field Characterization in a Bridgman Apparatus:</i>	
<i>Technique Development and Effect Analysis (Dr. Soyoung S. Cha).....</i>	813
<i>Microgravity Chemical Vapor Deposition (Dr. Ivan O. Clark).....</i>	815
<i>Glass Formation and Nucleation in Microgravity: Containerless-Processed,</i>	
<i>Inviscid Silicate/Oxide Melts (Ground-Based Studies) (Dr. Reid F. Cooper).....</i>	817
<i>Fundamental Studies of Solidification in Microgravity using Real-Time</i>	
<i>X-Ray Microscopy (Dr. Peter A. Curreri).....</i>	819
<i>Directional Solidification in 3He-4He Alloys (Prof. Arnold Dahm).....</i>	821
<i>Adaptive-Grid Methods for Phase Field Models of Microstructure</i>	
<i>Development (Dr. Jonathan A. Dantzig).....</i>	823
<i>Atomistic Simulations of Cadmium Telluride: Toward Understanding the</i>	
<i>Benefits of Microgravity Crystal Growth (Dr. Jeffrey J. Derby).....</i>	825
<i>Use of Synchrotron White Beam X-ray Topography for the Characterization</i>	
<i>of the Microstructural Development of Crystal - Normal Gravity Versus</i>	
<i>Microgravity (Dr. Michael Dudley).....</i>	827
<i>Combined Synchrotron White Beam X-Ray Topography and High Resolution Triple</i>	
<i>Axis X-Ray Diffraction Characterization and Analysis of Crystals Grown in</i>	
<i>Microgravity and Ground Based Experiments (Dr. Michael Dudley).....</i>	830
<i>Reverse Micelle Based Synthesis of Microporous Materials in</i>	
<i>Microgravity (Prof. Prabir K. Dutta).....</i>	834
<i>Reverse Micelle Based Synthesis of Microporous Materials in</i>	
<i>Microgravity (Prof. Prabir K. Dutta).....</i>	836
<i>Studies on Nucleation, Polymerization, and Nanoparticle Composites in</i>	
<i>Supersaturated Vapors under Microgravity Conditions (Dr. M. S. El-Shall).....</i>	837
<i>Theoretical and Experimental Investigation of Vibrational Control of the</i>	
<i>Bridgman Crystal Growth Technique (Dr. Alexandre I. Fedoseyev).....</i>	839
<i>The Impaction, Spreading, and Solidification of a Partially Solidified</i>	
<i>Undercooled Drop (Dr. Merton C. Flemings).....</i>	841
<i>Investigation of Local Effects on Microstructure Evolution (Dr. Donald O. Frazier).....</i>	843
<i>Melt Stabilization of PbSnTe in a Magnetic Field (Dr. Archibald L. Fripp).....</i>	845
<i>Solidification of II-VI Compounds in a Rotating Magnetic Field (Dr. Donald C. Gillies).....</i>	847
<i>Electronic Materials (Mr. Thomas K. Glasgow).....</i>	849
<i>Effect of Gravity on the Evolution of Spatial Arrangement of Features in</i>	
<i>Microstructure: A Quantitative Approach (Prof. Arun M. Gokhale).....</i>	850
<i>Evolution of Microstructural Distance Distributions in Normal Gravity and</i>	
<i>Microgravity (Prof. Arun M. Gokhale).....</i>	852
<i>Plasma Dust Crystallization (Dr. John A. Goree).....</i>	854

<i>Utilizing Controlled Vibrations in a Microgravity Environment to Understand and Promote Microstructural Homogeneity during Floating-Zone Crystal Growth</i> (Dr. Richard N. Grugel).....	856
<i>Novel Directional Solidification Processing of Hypermonotectic Alloys</i> (Dr. Richard N. Grugel).....	858
<i>Influence of Free Convection in Dissolution</i> (Prof. Prabhat K. Gupta).....	859
<i>Microgravity Processing of Oxide Superconductors</i> (Dr. William H. Hofmeister).....	860
<i>Dimensional Stability of Supermatrix Semiconductors</i> (Dr. Douglas E. Holmes).....	862
<i>Non-Equilibrium Phase Transformations</i> (Dr. Kenneth A. Jackson).....	864
<i>Dislocation Formation during Growth of Semiconductor Crystals</i> (Dr. Monica L. Kaforey).....	866
<i>The Role of Dynamic Nucleation at Moving Boundaries in Phase and Microstructure Selection</i> (Dr. Alain S. Karma).....	867
<i>Identification of Gravity-Related Effects on Crystal Growth from Melts with an Immiscibility Gap</i> (Dr. Mohammad Kassemi).....	869
<i>Combined Heat Transfer Analysis of Crystal Growth</i> (Dr. Mohammad Kassemi).....	871
<i>Measurement of Liquid-to-Solid Nucleation Rates in Undercooled Metallic Melts</i> (Dr. Joseph L. Katz).....	873
<i>Fundamentals of Thermomigration of Liquid Zones Through Solids</i> (Prof. Michael J. Kaufman).....	875
<i>Compositional Dependence of Phase Formation and Stability</i> (Dr. Kenneth F. Kelton).....	877
<i>Phase Formation and Stability: Composition and Sample-Size Effects</i> (Dr. Kenneth F. Kelton).....	879
<i>Solutocapillary Convection Effects on Polymeric Membrane Morphology</i> (Dr. William B. Krantz).....	881
<i>Influence of Natural Convection and Thermal Radiation on Multi-Component Transport and Chemistry in MOCVD Reactors</i> (Dr. Anantha Krishnan).....	883
<i>Containerless Property Measurement of High-Temperature Liquids</i> (Dr. Shankar Krishnan).....	885
<i>Noise and Dynamical Pattern Selection in Solidification</i> (Prof. Douglas A. Kurtze).....	887
<i>Study of Magnetic Damping Effect on Convection and Solidification under G-Jitter Conditions</i> (Dr. Ben Q. Li).....	888
<i>Microstructural Development during Directional Solidification of Peritectic Alloys</i> (Dr. Thomas A. Lograsso).....	890
<i>Numerical Investigation of Thermal Creep and Thermal Stress Effects in Microgravity Physical Vapor Transport</i> (Dr. Daniel W. Mackowski).....	892
<i>Polymerizations in Microgravity: Traveling Fronts, Dispersions, Diffusion and Copolymerizations</i> (Dr. Lon J. Mathias).....	894

<i>Quantitative Analysis of Crystal Defects by Triple Crystal X-Ray Diffraction</i> (Dr. Richard J. Matyi).....	897
<i>Numerical and Laboratory Experiments on the Interactive Dynamics of Convection, Flow, and Directional Solidification</i> (Prof. Tony Maxworthy).....	899
<i>The Interactive Dynamics of Convection, Flow and Directional Solidification</i> (Prof. Tony Maxworthy).....	901
<i>Y2BaCuO5 Segregation in YBa2Cu3O7-x During Melt Texturing</i> (Dr. Paul J. McGinn).....	903
<i>Interaction of Hele-Shaw Flows with Directional Solidification: Numerical Investigation of the Nonlinear Dynamical Interplay and Control Strategies</i> (Prof. Eckart H. Meiburg).....	905
<i>The Synergistic Effect of Ceramic Materials Synthesis Using Vapor-Enhanced Reactive Sintering Under Microgravity Conditions</i> (Prof. John J. Moore).....	907
<i>Diffusion, Viscosity, and Crystal Growth in Microgravity</i> (Dr. Allan S. Myerson).....	909
<i>An Electrochemical Method to Measure Diffusivity in Liquid Metals</i> (Prof. Ranga Narayanan).....	911
<i>Crystal Growth and Segregation Using the Submerged Heater Method</i> (Dr. Aleksandar G. Ostrogorsky).....	913
<i>Gravitational Effects on the Morphology and Kinetics of Photo-Deposition of Polydiacetylene Films from Monomer Solutions</i> (Dr. Mark S. Paley).....	915
<i>Investigation of "Contactless" Crystal Growth by Physical Vapor Transport</i> (Dr. Witold Palosz).....	917
<i>Investigation of Convective Effects in Crystals Growth by Physical Vapor Transport</i> (Dr. Witold Palosz).....	919
<i>Containerless Processing of Composite Materials</i> (Prof. John H. Perepezko).....	920
<i>Analysis of Containerless Processing and Undercooled Solidification Microstructures</i> (Prof. John H. Perepezko).....	922
<i>Containerless Processing for Controlled Solidification Microstructures</i> (Prof. John H. Perepezko).....	924
<i>Comparison of the Structure and Segregation in Dendritic Alloys Solidified in Terrestrial and Low Gravity Environments</i> (Prof. David R. Poirier).....	926
<i>The Effects of Microgravity on Vapor Phase Sintering</i> (Prof. Dennis W. Readey).....	928
<i>Modeling of Detached Solidification</i> (Dr. Liya L. Regel).....	932
<i>Thermophysical Property Measurement of Molten Semiconductors in 1-g and Reduced-g Conditions</i> (Dr. Won-Kyu Rhim).....	934
<i>Undercooling Limits and Thermophysical Properties in Glass Forming Alloys</i> (Dr. Won-Kyu Rhim).....	936
<i>Drop Tube Operation</i> (Dr. Michael B. Robinson).....	938

<i>Measurement of the Optical and Radiative Properties of High-Temperature Liquid Materials by FTIR Spectroscopy (Dr. Michael B. Robinson).....</i>	940
<i>Undercooling Behavior of Immiscible Metal Alloys in the Absence of Crucible Induced Nucleation (Dr. Michael B. Robinson).....</i>	941
<i>A Study of the Undercooling Behavior of Immiscible Metal Alloys in the Absence of Crucible-Induced Nucleation (Dr. Michael B. Robinson).....</i>	942
<i>Determination of the Surface Energy of Liquid Crystals from the Shape Anisotropy of Freely Suspended Droplets (Dr. Charles S. Rosenblatt).....</i>	944
<i>Modeling of Macroscopic/Microscopic Transport & Growth Phenomena in Zeolite Crystal Solutions under Microgravity (Dr. Albert Sacco).....</i>	946
<i>Undercooling Limits in Molten Semiconductors and Metals: Structure and Superheating Dependencies (Prof. Frank G. Shi).....</i>	947
<i>Gravitational Effect on the Development of Laser Weld-Pool and Solidification Microstructure (Dr. Jogender Singh).....</i>	948
<i>Flight Experiment to Study Double Diffusive Instabilities in Silver-Doped Lead Bromide Crystals (Dr. N. B. Singh).....</i>	950
<i>Double Diffusive Convection during Growth of Lead Bromide Crystals (Dr. N. B. Singh).....</i>	953
<i>Kinetics of Nucleation and Growth from Undercooled Melts (Prof. Frans A. Spaepen).....</i>	955
<i>Crystal Nucleation, Hydrostatic Tension, & Diffusion in Metal and Semiconductor Melts (Prof. Frans A. Spaepen).....</i>	958
<i>Micro- and Macro-Segregation in Alloys Solidifying with Equiaxed Morphology (Dr. Doru M. Stefanescu).....</i>	961
<i>Test of Magnetic Damping of Convective Flows in Microgravity (Dr. Frank R. Szofran).....</i>	963
<i>Magnetic Damping of Solid Solution Semiconductor Alloys (Dr. Frank R. Szofran).....</i>	965
<i>The Features of Self-Assembling Organic Bilayers Important to the Formation of Anisotropic Inorganic Materials in Microgravity Conditions (Dr. Daniel R. Talham).....</i>	967
<i>Microporous Membrane and Foam Production by Solution Phase Separation: Effects of Microgravity and Normal Gravity Environments on Evolution of Phase Separated Structures (Dr. John M. Torkelson).....</i>	969
<i>Dynamically-Induced Nucleation of Deeply Supercooled Melts and Measurement of Surface Tension and Viscosity (Dr. Eugene H. Trinh).....</i>	972
<i>A Proposal to Further Investigate the Influence of Microgravity on Transport Mechanisms in a Virtual Space Flight Chamber (Dr. James D. Trolinger).....</i>	974
<i>Fundamentals of Mold-Free Casting Experimental and Computational Studies (Prof. Grétar Tryggvason).....</i>	976
<i>Electromagnetic Field Effects in Semiconductor Crystal Growth (Dr. Martin P. Volz).....</i>	978

<i>Models of Magnetic Damping for Semiconductor Crystal Growth in Microgravity</i> (Dr. John S. Walker).....	980
<i>Process-Property-Structure Relationships in Complex Oxide Melts</i> (Dr. Richard Weber).....	982
<i>Thin Film Mediated Phase Change Phenomena: Crystallization, Evaporation and Wetting</i> (Prof. John S. Wettlaufer).....	985
<i>Defect Generation in CVT Grown Hg_{1-x}Cd_xTe Epitaxial Layers under Normal and Reduced Gravity Conditions</i> (Dr. Heribert Wiedemeier).....	987
<i>Use of Microgravity to Control the Microstructure of Eutectics</i> (Dr. William R. Wilcox).....	988
<i>BSO/BTO Identification of Gravity Related Effects on Crystal Growth, Segregation, and Defect Formation</i> (Dr. August F. Witt).....	990

Advanced Technology Development

<i>Free Float Trajectory Management ATD</i> (Mr. A. P. Allan).....	992
<i>Low Temperature Magnetostrictive Smart Actuator Mechanisms</i> (Dr. Robert G. Chave).....	994
<i>Real-Time X-Ray Microscopy for Solidification Processing</i> (Dr. Peter A. Curreri).....	996
<i>Single Electron Transistor (SET)</i> (Dr. Pierre Echternach).....	998
<i>Advanced Heat Pipe Technology for Furnace Element Design</i> (Dr. Donald C. Gillies).....	1000
<i>Space Bioreactor Bioproduct Recovery System</i> (Steve R. Gonda, Ph.D.).....	1002
<i>Microgravity Combustion Diagnostics</i> (Mr. Paul S. Greenberg).....	1004
<i>High Resolution Pressure Transducer and Controller</i> (Dr. Ulf E. Israelsson).....	1013
<i>Surface Fluctuation Spectrometers for the Characterization of Fluid and Crystal Surfaces</i> (Mr. William V. Meyer).....	1015
<i>The Laser Feedback Interferometer: A New, Robust, and Versatile Tool for Measurements of Fluid Physics Phenomena</i> (Dr. Ben Ovryn).....	1018
<i>Crystal Growth Instrumentation Development: A Protein Crystal Growth Studies Cell</i> (Dr. Marc L. Pusey).....	1020
<i>High Resolution Thermometry and Improved SQUID Readout</i> (Dr. Peter Shirron).....	1023
<i>Passive Free Vortex, Two-Phase Separator</i> (Dr. J. M. Shoemaker).....	1025
<i>Determination of Soot Volume Fraction Using Laser-Induced Incandescence</i> (Dr. Randall L. Vander Wal).....	1027
<i>Ceramic Cartridges via Sintering and Vacuum Plasma Spray</i> (Mr. Frank R. Zimmerman).....	1030

Technology Transfer

<i>Advanced High Brilliance X-Ray Source</i> (Dr. Daniel C. Carter).....	1031
--	------

Interagency Agreements

<i>NASA/NIH Inter-agency Agreement</i> (Dr. Joshua Zimmerberg, NIHCD).....	1033
--	------

IV. BIBLIOGRAPHY	III-1055
------------------------	----------

APPENDIX

Appendix A: Table of Acronyms	A-1
Appendix B: Guest Investigator Index	B-1
Appendix C: Principal Investigator Index	C-1

I. Introduction

- **Objectives and Focus for FY1996 I-3**
- **Program Task Summary Data I-5**
- **Principal Investigator Distribution Map I-6**

OBJECTIVES AND FOCUS FOR FY1996

NASA's Microgravity Science and Applications Division (MSAD) sponsors a program that expands the use of space as a laboratory for the study of important physical, chemical, and biochemical processes. The primary objective of the program is to broaden the value and capabilities of human presence in space by exploiting the unique characteristics of the space environment for research. However, since flight opportunities are rare and flight research development is expensive, a vigorous ground-based research program, from which only the best experiments evolve, is critical to the continuing strength of the program.

The microgravity environment affords unique characteristics that allow the investigation of phenomena and processes that are difficult or impossible to study on Earth. The ability to control gravitational effects such as buoyancy driven convection, sedimentation, and hydrostatic pressures make it possible to isolate phenomena and make measurements that have significantly greater accuracy than can be achieved in normal gravity. Space flight gives scientists the opportunity to study the fundamental states of physical matter—solids, liquids and gasses—and the forces that affect those states. Because the orbital environment allows the treatment of gravity as a variable, research in microgravity leads to a greater fundamental understanding of the influence of gravity on the world around us. With appropriate emphasis, the results of space experiments lead to both knowledge and technological advances that have direct applications on Earth. Microgravity research also provides the practical knowledge essential to the development of future space systems.

The Office of Life and Microgravity Sciences and Applications (OLMSA) is responsible for planning and executing research stimulated by the Agency's broad scientific goals. OLMSA's Microgravity Science and Applications Division (MSAD) is responsible for guiding and focusing a comprehensive program, and currently manages its research and development tasks through five major scientific areas: biotechnology, combustion science, fluid physics, fundamental physics, and materials science.

FY 1996 was an important year for MSAD. NASA continued to build a solid research community for the coming space station era. During FY 1996, the NASA Microgravity Research Program continued investigations selected from the 1994 combustion science, fluid physics, and materials science NRAs. MSAD also released a NASA Research Announcement in microgravity biotechnology, with more than 130 proposals received in response. Selection of research for funding is expected in early 1997. The principal investigators chosen from these NRAs will form the core of the MSAD research program at the beginning of the space station era.

The third United States Microgravity Payload (USMP-3) and the Life and Microgravity Spacelab (LMS) missions yielded a wealth of microgravity data in FY 1996. The USMP-3 mission included a fluids facility and three solidification furnaces, each designed to examine a different type of crystal growth. USMP-3 saw the second successful flight of the Critical Fluid Light Scattering Experiment/Zeno, and the Isothermal Dendritic Growth Experiment (IDGE) became the first US microgravity experiment to be commanded and controlled from the principal investigator's university. Research aboard the LMS in biotechnology, fluid physics, and materials science allowed US investigators to use instruments developed by the European Space Agency (ESA), thus broadening the basis for international cooperation in space research. The LMS mission was the first to fly the ESA-developed Advanced Gradient Heating Furnace (AGHF). During FY 1996 the biotechnology program supported 20 experimental instrument flights in protein crystal growth and cell science, with more than

1500 protein samples flown. The first long duration flight of a cell and tissue culturing device was placed in orbit in the Mir during FY 1996.

This document, NASA Technical Memorandum 4780 [1997], The Microgravity Science and Applications Program Tasks and Bibliography for Fiscal Year 1996 (October 1995 – September 1996), includes research projects funded by the Office of Life and Microgravity Sciences and Applications, Microgravity Science and Applications Division, during that year. This document is published annually and is sent to scientists in the microgravity research, both foreign and domestic. The information provided in the Task Book is used in reports within NASA, and to the Office of Management and Budget and the United States Congress.

The Microgravity Science and Applications Division wishes to thank Information Dynamics, Inc., and in particular recognize Mr. Bill Wilcox (task book review process and publications manager/editor) for his lead efforts in the development, compilation, and publishing of this report. Gratitude is also expressed for significant data processing support at the responsible Centers for MSAD task management, recognizing: Dr. Donald Strayer and Ms. Angela Belcastro, JPL; Ms. Phyllis Golden, JSC; Mrs. Mary Malone, LeRC; and Mr. Charles Walker, MSFC.

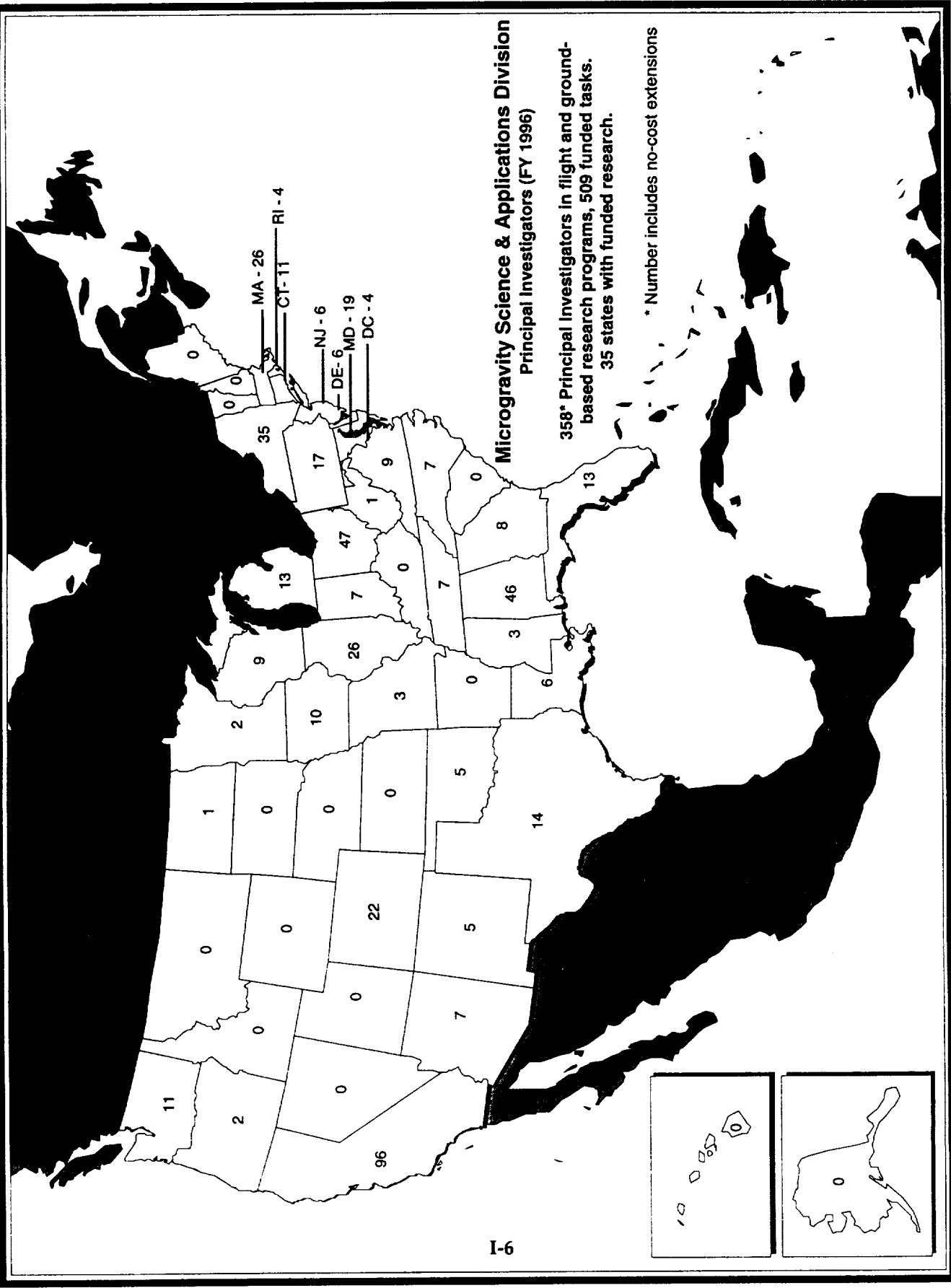
**FY1996 PROGRAM RESEARCH TASK SUMMARY:
Overview Information and Statistics**
Total Number of Principal Investigators: 358*
Total Number of Co-Investigators: 396
Total Number of Bibliographic Listings: 1,573

- Proceedings Papers: 237
- Journal Articles: 600
- NASA Tech Brief Articles: 14
- Science/Technical Presentations: 706
- Books/Chapters:..... 16

Total Number of Patents Applied for or Awarded: 2
Number of Graduate Students Funded: 780
Number of Graduate Degrees Granted
Based on MSAD-funded Research: 247
Number of States with Funded Research (including District of Columbia): 35
FY1995 Microgravity Science & Applications Budget: 159.0 Million

<i>Microgravity Science & Applications Research Tasks and Types — Responsibilities by Center —</i>				
Centers, Types of Research	Ground	Flight	ATD	Center Totals
Jet Propulsion Laboratory	45	7	3	55
Johnson Space Flight Center	32	1	1	34
Langley Research Center	2	1	0	3
Lewis Research Center	203	46	6	255
Marshall Space Flight Center	124	32	4	160
Goddard Space Flight Center	0	0	1	1
Research Task Totals	406	87	15	508

* Number includes no-cost extensions



II. Microgravity Science & Applications Program Tasks for FY 1996

- **Flight Research Tasks**
 - Biotechnology II-9
 - Combustion Science II-25
 - Fluid Physics II-75
 - Fundamental Physics II-127
 - Materials Science II-137
- **Ground Research Tasks**
 - Biotechnology II-197
 - Combustion Science II-346
 - Fluid Physics II-454
 - Fundamental Physics..... II-706
 - Materials Science II-770
- **ATD**
 - Advanced Technology Development II-992
- **Technology Transfer**.....II-1031
- **Interagency Agreements**..... II-1033

Protein Crystal Growth Vapor-Diffusion Flight Hardware and Facility

PRINCIPAL INVESTIGATOR: Dr. Daniel C. Carter

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Ho, J. (X. He)

NASA Marshall Space Flight Center (MSFC)

Miller, T.

NASA Marshall Space Flight Center (MSFC)

Task Objective:

The major objectives of this research are aimed at the design, construction, and operation of an improved microgravity protein crystal growth hardware and facility.

Task Description:

Previously, in response to the first NASA Biotechnology NRA, we proposed to develop and construct a facility based protein crystal growth concept. This was undertaken largely because of the many important examples of quality improvements gained from growth in the diffusion-limited environment in space. The concept was based on the adaptation for microgravity of a commonly used disposable crystallization tray thereby improving sample logistics and handling, as well as greatly increasing the potential co-investigator group and science return. The proposal proceeded in two phases, in the first stage a hand-held concept was to be developed and tested in microgravity to test the principle/concept. If successful, we further proposed to construct a facility for the mass production of protein crystals for application in the structure determination. Access to the facility is open to scientists from industry, academia and government laboratories. The principal aims of the research are:

- (1) Establish a protein crystal growth facility which would provide greatly increased experiment and co-investigator capacity in order to increase the odds of obtaining suitable crystals, consequently increasing the overall science return from each mission.
- (2) Investigate the disposable interface concept in development of microgravity hardware for reduced cost and improvements in logistics and handling.
- (3) Utilize the facility to delineate factors contributing to the effect of microgravity on the growth and quality of protein crystals.

Task Significance:

Improvements in the quality protein crystals can be the limiting step in the determination of the atomic structure. A detailed knowledge of the atomic three-dimensional structure of protein molecules is key to a fundamental understanding of biochemistry and is of tremendous application in structure-based drug design. Further, examination of crystals grown in microgravity provides important scientific data which illuminates the mechanisms involved in the growth of high quality crystals in the microgravity environment.

Progress During FY 1996:

During the course of this investigation hardware design and construction has proceeded rapidly through hand-held versions to complete facility hardware. A large flight co-investigator group has been established and the hardware has been manifested and flown successfully on several shuttle missions (see below). Additionally, special dialysis counter-diffusion hardware has been designed, constructed and is now currently active on *Mir*. The accomplishments from both the hardware development and the results from the flight experiments have been outstanding. Over the course of three flights of the PCAM facility hardware in 1995 over 1600 hundred individual vapor equilibration experiments were flown, exceeding the total number flown in the MSAD program since the inception of the protein crystal growth program in 1985. It should be noted that the PCAM hardware pioneered the development and deployment of disposable interface in flight hardware which has resulted in greatly reduced costs, as well as numerous additional advantages. Highlights of the PCAM and DCAM experiments include crystals of human antithrombin III (Dr. Mark Wardell, Washington University) which were of greatly improved quality. These crystals have allowed for the completion of the atomic model of this important protein. Improved crystals have also

been grown of neurophysin/vasopressin complex, liver augmenter (Dr. B.C. Wang, University of Georgia), raf kinase, lysozyme (Drs. J.P. Wery and David Clawson, Eli Lilly) and the nucleosome core particle (Dr. Gerry Bunick and Dr. Joel Harp, Oakridge National Laboratory). Several publications describing the improvements gained from microgravity are in preparation. 1996 marked the first long duration experiment for DCAM. Crystals produced from DCAM returned from STS-79 after a six month stay on Mir were recently distributed to the guest investigator group. Notable accomplishments include numerous, large spectacular crystals of the nucleosome core particle which were the largest grown to date (Dr. Gerry Bunick and Dr. Joel Harp, Oakridge National Laboratory) and the largest crystal ever produced of T7 RNA polymerase (Dr. B.C. Wang, University of Georgia). A summary for the flight experiments conducted to date are synopsized below. Several publications describing the effects and improvements gained in microgravity are in preparation.

Mission	Hardware	# sample chambers	# Investigators	# Proteins
STS-62	HH-PCAM	96	1	4
STS-63	6 PCAM	378	7 (5 groups)	9
STS-67	6 PCAM	378	11 (8 groups)	9
STS-73	12 PCAM	756	13 (8 groups)	12
	8 Short PCAM	168	1	
	81 DCAM	162	3	3
STS-76	162 DCAM	162	8 (7 groups)	9
STS-79	162 DCAM	81	9 (7 groups)	11

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/93 EXPIRATION: 11/97

PROJECT IDENTIFICATION: 963-45-08

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Carter, D.C. "PCAM and DCAM, Summary of Flight Results 1994-96." Protein Crystal Growth Workshop, Panama City Beach, Florida, May 1996.

Carter, D.C. "PCAM and DCAM, Summary of Flight Results 1995-96." Gordon Research Conference, New Hampshire, June 1996.

Carter, D.C. "PCAM and DCAM Hardware and Facility." International Microgravity Protein Crystal Growth Workshop, University of California, Riverside, 1996.

Protein Crystal Growth in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Lawrence J. DeLucas

University of Alabama, Birmingham

CO-INVESTIGATORS:see attached list (Appendix B)

Task Objective:

The objectives of this research are the following: to develop improved protein crystal growth flight hardware to produce larger, high quality protein crystals in microgravity for use in the determination of protein molecular structures for applications in medicine, drug design, agriculture, and the biological sciences; and to understand the dynamics/process of protein crystal growth.

Task Description:

Two laboratory based systems have been constructed to demonstrate methods which will allow for dynamic control of protein crystal growth. The technologies developed in these systems will be incorporated into future flight hardware for use in microgravity studies. The first system uses a precisely controlled vapor diffusion approach to monitor and control protein crystal growth. The system utilizes a humidity sensor and various interfaces under computer control to effect virtually any evaporation rate from up to 40 different growth solutions simultaneously. A static laser light scattering sensor can be used to detect aggregation events and trigger a change in the evaporation rate for a growth solution. The second system exploits the varying solubility of proteins versus temperature to control the growth of protein crystals. This system contains miniature thermoelectric devices under microcomputer control which change temperature as needed to grow crystals of a given protein. Complex temperature ramps are possible using this approach. A static laser light scattering probe is also included in this system as a non-invasive probe for detection of aggregation events. Both of these systems demonstrate significant advances in the ability of researchers to gain control of the protein crystal growth process and will provide tremendous opportunities for both terrestrial and microgravity research.

Task Significance:

Larger, high quality protein crystals may be used in molecular structure determinations for applications in medicine, drug design, agriculture, and the biological sciences.

Progress During FY 1996:**DCPCG - Vapor Diffusion**

Two systems were constructed which utilize vapor diffusion to control the nucleation and growth of protein crystals. These devices demonstrate that vapor diffusion can be successfully used to gain control over the crystal growth process in a manner previously unavailable. The first system demonstrates the effects of varying the evaporation rate on the size and number of the resulting crystals. This system can simultaneously vary the evaporation rate for up to 40 different experiments. This is achieved using humidity sensors, multiplexing of several chambers to one sensor, microcomputer control, and custom software. The second system incorporates a static laser light scattering system which is used as a sensor to detect aggregation events occurring in growth solutions and respond by changing the evaporation rate of one or more growth solutions. This system allows six chambers to be controlled dynamically in a Control/Follower configuration, with one chamber (Control) actively monitored with the light scattering system while the remaining chambers (Followers) are operated relative to the Control. These systems have shown that varying the evaporation rate of the growth solutions systematically affects the size and number of the crystals obtained. Faster evaporation rates generally lead to larger populations of smaller crystals than slower evaporation rates. Inclusion of a non-invasive sensor (LLS) has been used to detect crystals aggregation, at which point the initial evaporation rate is modified, resulting in a smaller population of larger crystals than obtained without dynamic response. These results are likely related to the length of time that a given growth solutions resides at a supersaturation level where nucleation occurs.

DCPCG - Temperature

A thermal temperature device was developed as a rapid qualitative screening method for the determination of temperature dependent solubility of proteins and for general screening of crystallization conditions for protein crystal growth. This device was used to assess the solubility of five proteins. Three of these proteins, hen egg albumin, alpha chymotrypsinogen A and equine serum albumin were observed to have a retrograde solubility while catalase and concanavalin A did not appear to have a temperature dependent solubility with respect to the parameters screened. It was demonstrated that static light scattering can be used to detect the aggregation of lysozyme and insulin and that the particle size response of these proteins to changes in temperature is rapid, thereby allowing a decoupling of the nucleation and growth stages of crystal growth. This DCPCG - Temperature method should facilitate the design of more efficient and successful crystal growth experiments.

The Center has just had the PDR for this program and is awaiting authorization to proceed.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 4/94 EXPIRATION: 3/98

PROJECT IDENTIFICATION: 963-55-01

NASA CONTRACT NO.: NAS8-401

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Bray, T.L., Powell, D.L., Kim, L.J., Gray, R.J., Le, T., Askew, R.P., Harrington, M.D., Rosenblum, W.M., Wilson, W.W., and DeLucas, L.J. New Crystallization Systems Envisioned for Microgravity Studies. J. Appl. Crystall., (1996, in revision).

Electrophoretic Separation of Cells and Particles from Rat Pituitary

PRINCIPAL INVESTIGATOR: Dr. Wesley C. Hymer

Pennsylvania State University

CO-INVESTIGATORS:

Mastro, A.
Grindeland, R.
Snyder, R.Pennsylvania State University
NASA Ames Research Center (ARC)
NASA Marshall Space Flight Center (MSFC)

Task Objective:

The objectives are to separate (1) pituitary cells and (2) hormone-containing granules by free flow electrophoresis using the Japanese Free-Flow Electrophoresis Unit (FFEU) on Earth and in space.

Task Description:

To accomplish these objectives it is necessary to: (1) optimize conditions for maintaining live pituitary cells in Japanese cell culture kits (CCK) for 21 days; (2) remove cells from the CCK in space and fractionate them by electrophoresis; and, (3) break open the cells in space and fractionate the lysate by electrophoresis to obtain hormone-containing granules. These procedures must be done in such a way as to be executable in flight. It is also necessary to modify existing technologies in order to analyze different hormone forms of growth hormone and prolactin in these fractions. Both hormones will be assayed by both immune and biological assays.

Because FY94 was the flight year for this experiment, the logistics associated with conducting pre-flight, flight, and post-flight operations was also required.

Task Significance:

- (1) Pituitary growth hormone and prolactin are required for proper function of the bone, muscle, and immune systems. Because these systems are modified by spaceflight, and because the results from four previous space experiments show that the biological activities of growth hormone and prolactin are diminished during and after spaceflight, this experiment is intended to probe the mechanism(s) by which these changes occur.
- (2) Biotechnology research on earth routinely utilizes coupled technologies to meet focused objectives. Coupled technologies are difficult to accomplish in a low gravity environment; yet these will be routine on Space Station Alpha. This experiment serves as a prototype for such activities.

Progress During FY 1996:

Two manuscripts describing the results of our experiment done on the IML-2 mission have been submitted to the Journal of Biotechnology and are currently in review. Key findings:

- (a) The frequencies of changing cell culture medium in microgravity affected the amount and activity of some, but not all, of the six pituitary hormones released into the medium.
- (b) Extensive cell clumping occurred in low gravity cultures without media change.
- (c) Fresh enzyme solutions prepared in microgravity successfully detached cells from their substrate; these reattached and retained function in low gravity.
- (d) Processing of a pituitary cell lysate, coupled to separation of its growth hormone containing particles by free flow electrophoresis, was successful.
- (e) Post-flight electrophoresis trials of microgravity-exposed pituitary cells showed that cell feeding frequency affected their net surface charge. This result was unique to low gravity.

Publications resulting from this research and the IML-2 flight experiment are in the final stages of completion. Specifically, two papers, which will appear in the J. of Biotechnology this fiscal year (and are in press) require shepherding through to publication. Finally, two additional manuscripts are in preparation for inclusion in the IML-2 brochure which will be published by NASA (MSFC) this fiscal year.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 12/89 **EXPIRATION:** 2/97

PROJECT IDENTIFICATION: 963-35-15

NASA CONTRACT No.: NAG8-953

RESPONSIBLE CENTER: MSFC

Growth, Metabolism, and Differentiation of MIP-101 Carcinoma Cells

PRINCIPAL INVESTIGATOR: Dr. J. M. Jessup

Harvard Medical School

Co-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Our objective is to determine whether the metabolism and differentiation of human colon carcinoma cells in actual microgravity is similar to that exhibited in simulated microgravity.

Task Description:

MIP-101 is a poorly differentiated human colon carcinoma that was initially established from the ascites of a patient with widely metastatic cancer. Previous work has found that these tumor cells do not produce carcinoembryonic antigen (CEA) or related molecules, are not metastatic, and grow as isolated cells in monolayer culture. However, growth in vivo in athymic nude mice induces the expression of CEA and similar proteins as well as increases the metastatic potential of MIP-101 cells. Growth in simulated microgravity in the RWV induces the expression of CEA and related proteins and may have an effect on metastatic potential. Our task is to assess whether growth of MIP-101 cells in the Biotechnology Specimen Container (BSTC) in actual microgravity also upregulates the expression of CEA and related proteins and changes the metabolic or cell cycle parameters of the cells.

Task Significance:

This work is important because it will define the effects of microgravity on the growth, metabolism, and differentiation of a human colon carcinoma cell line that is useful for microgravity research. Our preliminary ground-based experiments suggest that metabolism of MIP-101 is significantly increased in simulated microgravity and strains the capacity of the RWV to support its growth. This cell line will assess how aggressively cells consume nutrients in microgravity when three-dimensional culture is attempted under non-perfused conditions and will test the metabolic requirements of space-based bioreactors. As a result, there is a need to know whether microcarrier cultures produce three-dimensional cultures in space at the metabolic rate observed in the RWV. The MIP-101 cells are important for this test because they are the only cells which display differentiation (production of CEA and CEA-related proteins) as monocultures in the RWV. Finally, we may begin to realize the potential of microgravity to foster three-dimensional cultures and to produce growth and regulatory factors.

Progress During FY 1996:

During the first months of this grant, the MIP-101 cells which we have been using were flown in EDU-1 on Shuttle Mission STS-70. We had hoped that during the period of the next twelve months that there would be a reflight because we did not want to publish the findings of this first flight without first repeating it in order to assure ourselves that the results were valid as reported in last year's annual report. The performance of the bioreactor in actual microgravity was exactly as expected, and the number of cells produced, the metabolism of the cells, and the general morphological appearance was well maintained. The cells in microgravity did not demonstrate any apoptosis compared to the cells in the ground controls which had a 1-3% apoptotic rate.

Although we have not been able to have a reflight, we have focused on the cellular morphology and the fact that actual microgravity cultures more closely resemble static three-dimensional cultures of MIP-101 cells than did the ground controls. We have found that MIP-101 cells accumulate in G2/M in the Rotating Wall Vessel (RWV) compared to the same cells growing either as flat single cell monolayers or as multicellular spheroids in stationary, static 3-D culture. We have examined the molecular expression of various cell cycle regulatory proteins and have found that proteins associated with G2/M are altered. For a cell to go through G2 and traverse mitosis requires the activity of cyclin B and p34^{cdc2} as well as that of the phosphatase cdc25C. We have found that cyclin B protein levels are increased considerably and that the protein level of cdc25C is decreased. Our collaborator, Dr. E. Leof at the Mayo Clinic, has analyzed our samples and found that the kinase activities of cyclins A and E as well as p34^{cdc2} are markedly decreased in the RWV cultures. Since we have also found that MIP-101 cells do not contain detectable

P21^{WAF1} or p27^{Kip1}, cell cycle-dependent kinase inhibitors (cdki's), and the MIP-101 cells undergo nuclear fragmentation and degradation. These cells, by lacking p21^{WAF1} or p27^{Kip1}, do not undergo apoptosis.

As a result, we are carefully beginning to dissect the cell cycle regulatory proteins that govern the ability of a cell to replace its DNA and S phase and to pass through G2 and M. To date, our results suggest that there is a general decrease in the activity of these enzymes but without the appearance of a cdki. Whether this is a specific defect in cell cycle regulatory proteins or is the result of a more generalized defect in energy production within the cells in the RWV remains to be determined and is the focus of the next year's work in this particular project.

We hope that we will be able to have a reflight in the next funding period and that we will be able to publish our results.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 963-45-23-22

NASA CONTRACT NO.: NAG9-835

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Jessup, J.M., Goodwin, T.J., Garcia, R., and Pellis N.R. "STS-70: First Flight of EDU-1." Society for In Vitro Biology, San Francisco, CA, June 1996.

Membrane Transport Phenomena

PRINCIPAL INVESTIGATOR: Mr. Larry W. Mason

Lockheed Martin Astronautics

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The Membrane Transport Phenomena (MTP) investigation will elucidate the role of gravity in membrane mediated mass transport. There are three objectives in this study: (1) development of a Membrane Transport Apparatus (MTA) to contain and observe experimental fluids; (2) experimental research using the apparatus to measure the kinetics of mass transport (osmosis) using a variety of solutes and membranes; and, (3) analytical model development to enable computational predictions and reconcile the experimental data.

Task Description:

The Membrane Transport Apparatus (MTA) will be designed and developed along with associated instrumentation and analysis tools to measure the kinetics of membrane mediated transport phenomena. Experiments will be conducted using a variety of fluids to measure mass transport under conditions where the primary variable is the convective environment within the experimental fluids. There are two convective modes to be investigated: induced convection (+1g), and inhibited convection (-1g). The instrument will be incrementally upgraded to allow measurement of additional fluid properties, and the application of additional trans-membrane driving forces. The experimental results will be analyzed to determine differences between gravimetric orientations, leading to definition of experimental conditions where microgravity effects are likely. The relative influence of coupled transport effects will also be determined. A series of (DC-9 aircraft) microgravity tests are planned to optimize instrument geometry and fluid transfer conditions, and to assist in definition of flight instrument hardware configurations.

Task Significance:

The MTP investigation addresses how gravity influences fluid boundary layers that are associated with membranes, and how gravity affects membrane mediated mass transport processes. Membranes are present in many different systems: biological, physiological, chemical, and biotechnological. Prior microgravity experiments using individual cells in the Biorack (Shuttle D-1 mission), Biosatellite II, Salyut, Cosmos, and additional Shuttle missions have clearly shown that important cellular functions are altered in microgravity. Some of the alterations include cytoplasmic streaming (protozoa), membrane properties and proliferation (bacteria), intracellular composition (slime molds), photosynthesis, growth rate, and overall morphology (plant cells), aggregation and morphology (red blood cells), and cellular differentiation and gene expression (lymphocytes). The broad range of changes seen may be explained by an alteration in a fundamental mechanism that is common to all systems. Many of these observed cellular changes can be explained as consequences of altered mass transport due to increased thickness of fluid boundary layers associated with membranes.

Progress During FY 1996:

The Membrane Transport Apparatus (MTA) instrument has been designed, fabricated, and assembled. The MTA is essentially an instrumented membrane that includes subsystems for solute manipulation, precision measurement of trans-membrane mass flow kinetics, and visualization and acquisition of solute refractive index profiles. Interface electronics for the MTA have been developed to enable computerized control of fluid manipulations, autonomous experimental data acquisition, and calibration of sensor and refractometer subsystems. Software programs have been developed for calibration and modeling of the refractometer subsystem, for reduction and analysis of imaged refractive index profiles, and for analysis of the experimental kinetic data.

The MTA is currently being used in a series of experiments to characterize the mass transport kinetics for a variety of solutes, membrane types, and gravimetric orientations. These experiments are conducted in each of two gravimetric orientations: induced convection (+1g), and inhibited convection (-1g). In the inhibited convection orientation (-1g), a stably stratified boundary layer forms in association with the membrane that alters the mass transport kinetics. The formation of this boundary layer is clearly observable in the MTA, and the relative effects of membrane type and solute nature are being determined.

An analytical model of the transport dynamics in the MTA is under development. The MTP Analytical Model is a one dimensional model that is based on an explicit forward in time central in space (FTCS) finite difference algorithm that describe the MTA geometry. The initial and boundary conditions are determined by the experimental solutes, the membrane characteristics, and the total solution volumes in the MTA. The gravimetric orientation determines the solute convective environment, and dictates whether or not a boundary layer forms in association with the membrane and the associated dynamics. Work is currently underway to reconcile the MTP Analytical Model predictions with experimental results.

A Fluids Manipulation System (FMS) is under development for a planned series of DC-9 microgravity flight experiments. These experiments will assess candidate flight instrument MTA container geometries for completeness of filling and the propensity to trap bubbles in microgravity. The DC-9 flight experiments are planned for FY97.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/95 EXPIRATION: 11/98

PROJECT IDENTIFICATION: 963-45-10

NASA CONTRACT NO.: NAS8-406

RESPONSIBLE CENTER: MSFC

An Observable Protein Crystal Growth Flight Apparatus

PRINCIPAL INVESTIGATOR: Dr. Alexander McPherson, Jr.

University of California, Riverside

CO-INVESTIGATORS:

Koszelak, S.
Malkin, A.
Kuznetsov, Y.
Jenkins, G.
Wells, M.

University of California, Riverside
University of California, Riverside
University of California, Riverside
University of California, Riverside (Huntsville)
University of California, Riverside (Huntsville)

Task Objective:

The task objective is to initiate research and development efforts in the area of macromolecular crystal growth, and specifically focused on the direct observation of the relevant phenomena as they pertain to the design and ultimate flight of an observable protein crystal growth apparatus (OPCGA).

Task Description:

The experiment objective includes the identification and characterization of candidate biochemical systems that include proteins, nucleic acids, and viruses. It further includes the construction of an optical platform that would be suitable for detailed interferometric analysis of protein crystal growth experiments and the visualization of concentration fields, the time lapse microphotography of macromolecular crystals, and the further characterization of the mechanisms and fundamental parameters that determine the features of macromolecular crystal growth.

Task Significance:

The need for structural information on biological macromolecules is of paramount importance to the emerging field of biotechnology. Such information provides the basis for the rational design of pharmaceuticals, the determination of enzymatic mechanisms and the engineering of proteins to enhance or modify their function. The value of x-ray crystallography to provide structural information at atomic resolution is unsurpassed. This technique does, however, depend on the availability of crystals for the macromolecule under study, and furthermore, which possess a high degree of internal order and suitable size and shape to allow the accurate collection of x-ray diffraction data.

Typically, crystals grown in the earth's gravitational field suffer from one or more types of flaws which decrease the structural information that can be derived from them. These imperfections include the relatively simple, but nonetheless adverse, problem of intergrowth. In a 1-g field several crystals, which nucleate independently, sediment to the bottom of the growth chamber where they intergrow into a mass not suitable for x-ray diffraction analysis. Such intergrowth or the appearance of satellite crystals, which were earlier thought to occur by nucleation at the sides of defects in pre-existing crystals, have been shown to be almost exclusively due to the effects of sedimentation and intergrowth. The value of a microgravity environment for the elimination of sedimentation in the preparation of these crystals is obvious. Early experiments conducted on board the Space Shuttle clearly indicated such benefits. They also provided the impetus for other researchers to design experiments and procedures for mimicking the effect of microgravity in ground-based experiments. The development of methods for successfully growing protein crystals in gels is an example of such activities.

Progress During FY 1996:

Using atomic force microscopy (AFM), the major mechanisms responsible for the growth of protein and virus crystals were elucidated. Ultimately, molecular resolution was achieved which permitted delineation of the detailed sequence of events by which individual step edges formed and advanced. In addition, studies of crystals of the protein thaumatin permitted elucidation of the mechanism by which three-dimensional nuclei, and two-dimensional steps appear on growing crystal surfaces.

Also using AFM, a number of unexpected phenomena associated with macromolecular crystal growth were directly visualized. These included the incorporation of microcrystals by large growing crystals of canavalin and STMV, the

formation of inclusions, and the incorporation of foreign particles. In addition, a careful study of the nature, frequency, and mechanism of defect formation in protein and virus crystals was completed, as was a very precise analysis of the kinetics of thaumatin crystal growth.

The data from AFM, combined with previous studies using Michaelson interferometry, and quasi-elastic light scattering, provides a firm, fundamental basis for interpreting crystal growth data and observations in the future. These will be critical to understanding how microgravity effects the macromolecular crystal growth process.

A full up prototype of the OPCGA has now been constructed that includes the solid optics phase shift Mach-Zehnder interferometer and the color, time lapse video capabilities that are the heart of the system. Mechanical, electrical, and I/O functions have now been tested and integrated for the TES envelope. Prototype crystallization cells were tested in the HHDTC on three separate missions and were proven successful. In the laboratory it has been demonstrated that depletion zones in solution, around growing crystals of ADP, lysozyme, and STMV (a virus) can indeed be visualized under some conditions, even in earth's gravity. A Requirements Definition Review was held and approval to continue development of the OPCGA toward flight was granted.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	3	PhD Degrees:	3

TASK INITIATION: 5/93 EXPIRATION: 5/98

PROJECT IDENTIFICATION: 963-45-07

NASA CONTRACT NO.: NAS8-396

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Ban, N., and McPherson, A. The structure of satellite panicum mosaic virus at 1.9 Å resolution. *Nature Structural Biology*, vol. 2, no. 10, 882-890 (1995).

Ban, N., Day, J., Wang, X., Ferrone, S., and McPherson, A. Crystal structure of an anti-anti-idiotypic shows it to be self-complementary. *J. Mol. Biol.*, vol. 255, 617-627 (1996).

Ban, N., Larson, S.B., and McPherson, A. Structural comparison of the plant satellite viruses. *Virology*, vol. 214, 571-583 (1995).

Canady, M.A., Larson, S.B., Day, J., and McPherson, A. Crystal structure of turnip yellow mosaic virus. *Nat. Struc. Biol.*, vol. 3, no. 9, 771-781 (1996).

Cole, T., Kathman, A., Koszelak, S., and McPherson, A. Determination of the local refractive index for protein and virus crystals in solution by Mach-Zehnder interferometry. *Anal. Biochemistry*, vol. 231, 92-98 (1995).

Giegé, R., Drenth, J., Ducruix, A., Saenger, W., and McPherson, A. Crystallogensis of biological macromolecules. Biological, microgravity, and other physico-chemical aspects. *Prog. Crystal Growth and Charact.*, vol. 30, 237-281 (1995).

Harris, L.J., Skaletsky, E., and McPherson, A. Crystallization of intact Monoclonal antibodies. *Proteins*, vol. 23, 285-289 (1995).

Ko, T.-P., Williams, R., and McPherson, A. The crystal structure of a ribonuclease B + d(pA)₄ complex. *Acta Cryst.*, vol. D52, 160-164 (1996).

Land, T.A., Malkin, A.J., Kuznetsov, Yu.G., McPherson, A., and DeYoreo, J.J. Mechanisms of protein crystal growth: An atomic force microscopy study of Canavalin crystallization. *Phys. Rev. Letters*, vol. 75, no. 13, 2774-2777 (1995).

Malkin, A.J., Kuznetsov, Y.G., Glantz, W., and McPherson, A. Atomic force microscopy studies of surface morphology and growth kinetics in thaumatin crystallization. *J. Phys. Chem.*, vol. 100, 11736-11743 (1996).

Malkin, A.J., Kuznetsov, Yu.G., and McPherson, A. Incorporation of microcrystals by growing protein and virus crystals. *Proteins*, vol. 24, 247-252 (1996).

Malkin, A.J., Land, T.A., Kuznetsov, Yu.G., McPherson, A., and DeYoreo, J.J. Investigation of virus crystal growth by in situ atomic force microscopy. *Phys. Rev. Letters*, vol. 75, no. 13, 2778-2781 (1995).

Malkin, A.J., Kuznetsov, Yu.G., Land, T.A., DeYoreo, J.J., and McPherson, A. Mechanisms of growth for protein and virus crystals. *Nature Structural Biology*, vol. 2, no. 11, 956-959 (1995).

Presentations

McPherson, A. "Nature and Effects of Impurities in Macromolecular Crystals." ICCBM Conference, Hiroshima University, Hiroshima City, Japan, November 12-17, 1995.

McPherson, A. "Macromolecular Crystal Growth in Microgravity." 6th International Space Conference of Pacific Basin Societies, Los Angeles, California, December 6-8, 1995.

McPherson, A. "Macromolecular Crystal Growth in Microgravity." 1st Conference on Commercial Development of Space - Space Technology & Applications Forum (STAIF 96), Albuquerque, New Mexico, January 7-11, 1996.

McPherson, A. "Presentation of Research and Hardware Development Plans FOR ISS-PCG (NASA MSFC)." International Workshop on Microgravity Biotechnology for the International Space Station (ISS), University of California - Riverside Campus, February 15-16, 1996.

McPherson, A. "Defect Structure and Density in Macromolecular Crystals." Protein Crystal Growth Conference, Panama Beach City, Florida, April 28-30, 1996.

McPherson, A. "The Nucleation Phase in Macromolecular Crystallization." International Meeting on Recent Advances in Macromolecular Crystallization, Bischoffsberg, France, June 2-4, 1996.

McPherson, A. "Macromolecular Crystal Growth in Microgravity." World Congress on In Vitro Biology, San Francisco, California, June 22-27, 1996.

McPherson, A. "Macromolecular Crystallization." IUCr XVII Congress and General Assembly, Seattle, Washington, August 8-17, 1996.

Enhanced Dewar Program

PRINCIPAL INVESTIGATOR: Dr. Alexander McPherson, Jr.

University of California, Riverside

CO-INVESTIGATORS:

Koszelak, S.

University of California, Riverside (UCR)

Jenkins, G.

University of California, Riverside (UCR)(Huntsville)

Task Objective:

The objective of the research is to develop a microgravity suitable system for screening protein crystallization conditions using the batch and liquid-liquid crystallization method.

Task Description:

Initially, a relatively simple system composed of a Dewar flask filled with small crystallization samples will be frozen on Earth and allowed to passively thaw in microgravity. Samples will be housed in the Passive GN₂ Freezer, a Dewar previously used in other microgravity applications. In addition to the crystallization experiments, plans are outlined for examination of crystals by standard light microscopy and also electron microscopy and atomic force microscopy, and detailed documentation of results, structure determination and high resolution refinement, and detailed analyses of structures obtained from crystals grown on Earth and in microgravity.

Task Significance:

These experiments represent an exciting and important new opportunity for protein crystal growth studies in microgravity. The proteins and protein solutions that will tolerate the freeze-thaw mechanism used to initiate these experiments will increase as the trend away from exclusion of glycerol from protein solutions used in crystallization continues. Shuttle experiments, furthermore, suggest that most orbiting platforms have some variations in the acceleration environment, and some protein crystallizations are more tolerant of these variations than others. Many of the difficulties that have affected most previous microgravity experiments can be circumvented in the Dewar system and long duration flights making possible crystallization experiments that cover much longer equilibration times.

Progress During FY 1996:

Results from three separate missions, each of duration 100-120 days, were obtained and analyzed. Of twenty-one different protein and virus samples whose crystallization was attempted, all twenty-one were obtained in crystal form on at least one mission. The first mission yielded seventeen successes in nineteen samples attempted.

In addition to the crystals, evidence was obtained suggesting that increased diffusion path lengths would be better suited to the Mir environment and the long duration. As a result of observations from the first two missions, diffusion tubes of double length were included on the third mission which has, at this writing, not yet returned from space.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 3/95 EXPIRATION: 3/99

PROJECT IDENTIFICATION: 963-45-07

NASA CONTRACT No.: NCC8-80

RESPONSIBLE CENTER: MSFC

Investigation of Protein Crystal Growth Mechanisms in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Keith B. Ward

Naval Research Laboratory (NRL)

CO-INVESTIGATORS:

Zuk, W.M.

Geo-Centers, Inc./Naval Research Laboratory (NRL)

Task Objective:

The objective of this program is to conduct flight experiments aimed at gathering fundamental data about how the processes of protein crystallization differ in a microgravity environment compared to unit gravity. The goals of these experiments therefore differ from those conducted by previous investigators who have limited their experiments to the preparation of large crystals suitable for x-ray diffraction analyses. The experiments performed under this project will be conducted in identical apparatuses both in ground-based and flight-based experiments. They will provide invaluable data about how solubility curves, nucleation kinetics, and crystal growth rates differ between microgravity and unit gravity. This information will then be used in the same apparatus to optimize conditions so as to favor the preparation of large, well ordered, single crystals. These results will prove crucial for the design of future generations of protein crystallization facilities that will be flown on a variety of space platforms.

Task Description:

The experiments will be conducted using the Canadian-American Telerobotic Crystallization Hardware (CATCH), a modified version of an apparatus developed under the auspices of the Canadian Space Agency. This equipment provides either liquid-liquid diffusion or mixed batch protocols, and incorporates a unique mixing mechanism that overcomes the difficulties encountered by current flight-based crystallization devices. The system also provides for monitoring light scattering signals from automated growth cells, allows video observation of the cells during the course of the experiments, and provides for precisely adjusting the growth cell temperature as a means of controlling protein supersaturation.

The automation system, which includes the flight computer and hardware interfaces of CATCH and the software necessary to control the apparatus, will be developed in the PI's laboratory as part of this project. Because of its ability to control the temperature and to monitor the progress of crystallization, CATCH will provide investigators the opportunity to devise experiments using dynamic control in which crystallization parameters are changed during the course of the experiments, either through predetermined experimental protocols or via commands provided by ground-based investigators. This unique ability to dynamically control the crystallization conditions is not afforded by any current microgravity crystallization device.

Task Significance:

Using CATCH, we will initiate a new series of flight experiments not limited to the preparation of single protein crystals, but which will also include the acquisition of fundamental data required to address the question of how microgravity may best be used to advantage in the preparation of such crystals. CATCH will allow investigators to monitor the results of crystallization trials, and more importantly, to reinitiate experiments based upon the nucleation and crystallization behavior observed in growth cells during the same flight. This use of telerobotic control inherent in CATCH will provide investigators an unparalleled level of efficiency in conducting microgravity crystallization experiments.

Progress During FY 1996:

We have developed a simple remote control system in our laboratory which can demonstrate an ability to operate crystallization experiments telerobotically. The laboratory-based system can be used to monitor remotely the progress of a crystallization experiment, and provides users on the Internet the ability to control the monitoring camera. The remote control demonstration may be accessed on the World Wide Web (WWW) and allows users to interact with control software located on our Web Server computer (<http://catch-www.nrl.navy.mil>). The user may position a video camera above a crystallization plate, capture a video image of the well, and observe the contents of the well on the Web page.

We have also begun conducting temperature controlled experiments using novel dynamic light scattering methods to examine the levels of aggregation of proteins both in bulk solution and close to various faces of a protein crystal. This information may be useful in understanding how proteins attach to a crystal face.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/95 EXPIRATION: 7/98

PROJECT IDENTIFICATION: 963-45-09

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Gorti, S., Zuk, W.M., Ward, K.B., Tanaka, T., and Yang, H. "Lysozyme Diffusion in the Vicinity of Crystal Surfaces."

Zuk, W.M., Gorti, S., and Ward, K.B. "Investigation of Protein Crystal Growth Mechanisms in Microgravity." Annual Protein Crystal Growth Conference, Panama City, Florida, April 28-30, 1996.

Scientific Support for an Orbiter Middeck Experiment on Solid Surface Combustion

PRINCIPAL INVESTIGATOR: Prof. Robert A. Altenkirch

Washington State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this flight experiment is to determine the controlling mechanisms of flames spreading over solid fuels in the absence of buoyant or externally imposed, gas-phase flows. Ground-based testing of flame spreading in quiescent microgravity environments has identified the qualitative importance of radiative heat losses in determining flame spread rates, but these tests are too short in duration to establish spreading flames without residual effects of the ignition process.

Task Description:

The Solid Surface Combustion Experiment (SSCE) was built to perform a minimum of eight flight experiments. The experiments are to consist of five flame spreading tests using a thin fuel, varying the atmospheric composition and pressure, then three additional tests using a thick fuel with fewer variations of the same parameters. In these tests, measurements of the fuel and flame temperature are to be made and recorded, and the flames are to be photographed, using motion picture film. A parallel effort is to be made to develop a complex numerical model of the opposed-flow flame spread problem, including the important effects of surface and gas-phase radiative losses. Finally, a detailed, quantitative comparison of experimental and computed results for flame spreading over thin and thick fuels in various oxidizer and pressure environments is to be performed including comparisons of spread rate, temperature and heat transfer fields and the structure of the flame.

Task Significance:

The spreading of flames over solid fuels is a fundamental combustion problem that has practical significance in the prevention and control of fires. Flame spreading in normal gravity is usually dominated by buoyant air flow that introduces a significant complexity into the fundamental models of the phenomena. Experiments conducted in the microgravity environment nearly eliminate this complexity, providing a more fundamental scenario for the development of flame spreading theory.

Progress During FY 1996:

1) The Solid Surface Combustion Experiment (SSCE) flight program was completed during the previous year. The primary focus of the efforts during this year were to conduct detailed comparisons of the flight results to the extensive numerical modeling results, including both steady and unsteady flame spreading calculations. The results of the last three flight experiments were presented at the 26th International Combustion Symposium.

2) The results of the Solid Surface Combustion Experiment are summarized briefly as follows:

A. Flame spreading is possible in an entirely quiescent environment, a result which is only possible to demonstrate in microgravity where buoyancy is removed. The minimum atmospheric oxygen concentration required to sustain spreading flames in a quiescent microgravity environment is higher than in normal gravity.

B. Flames over thin fuels can spread at a steady speed in quiescent microgravity, though the flame away from the leading edge where spreading occurs may be unsteady and grow or shrink.

C. Flames over thick fuels are inherently unsteady in quiescent environments and will eventually quench, though this quenching may occur long after ignition (measured in minutes).

D. Radiative heat transfer from the flame and the fuel surface must be considered in order to approach an accurate prediction of flame spreading behavior in quiescent environments. As the air flow velocity in the vicinity of the spreading flame is reduced, the fraction of heat released by the flame that is lost due to radiation becomes the dominant physical mechanism.

3) Funding of this program was completed during this year. A follow-on effort is reported under a different task entitled, "Reflight of the Solid Surface Combustion Experiment with Emphasis on Flame Radiation Near Extinction."

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	4	MS Degrees:	8
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 12/84 EXPIRATION: 12/96

PROJECT IDENTIFICATION: 963-22-05-01

NASA CONTRACT NO.: NAS3-239

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Bhattacharjee, S., Altenkirch, R.A., and Sacksteder, K.R., The effect of ambient pressure on flame spread over thin cellulosic fuel in a quiescent, microgravity environment. J. Heat Transfer, vol. 118, pp.181-190 (1996).

Presentations

Bhattacharjee, S., West, Altenkirch, R.A., "Determination of the spread rate in opposed-flow flame spread over thick solid fuels in the thermal regime." presented at the 26th International Symposium on Combustion, Naples Italy, 1996.

Delichatsios, M., "Creeping flame spread: energy balance and applications to practical materials." presented at the 26th International Symposium on Combustion, Naples Italy, 1996

West, Tang, Altenkirch, R.A., Bhattacharjee, S., Sacksteder, K., and Delichatsios, M., "Quiescent flame spread over thick fuels in microgravity." presented at the 26th International Symposium on Combustion, Naples Italy, 1996.

Low-Velocity, Opposed-Flow Flame Spread in a Transport-Controlled, Microgravity Environment

PRINCIPAL INVESTIGATOR: Prof. Robert A. Altenkirch

Washington State University

CO-INVESTIGATORS:

Bhattacharjee, S.
Olson, S.L.San Diego State University
NASA Lewis Research Center (LeRC)

Task Objective:

The overall objectives of the proposed work are to uncover the underlying physics and increase the fundamental understanding of the mechanisms that cause flames to propagate over solid fuels against a low velocity flow of oxidizer in the low-gravity environment. Although the work is fundamental in nature, it has clear applications to fire safety in space and on Earth. Specific objectives are:

1. To analyze experimentally observed flame shapes, measured gas-phase field variables, spread rates, radiative characteristics, and solid-phase regression rates for comparison with theoretical prediction capability previously developed that will be continually extended.
2. To investigate the transition from ignition to either flame propagation or extinction in order to determine the characteristics of those environments that lead to flame evolution.

Task Description:

To meet the objectives of the research program, a series of experiments has been developed to exercise several of the dimensional, controllable variables that affect the flame spread process in microgravity. Those variables that will be changed from experiment to experiment are the opposing flow velocity (1-20 cm/s), the external radiant flux directed to the fuel surface (0-2 W/cm²), and the oxygen concentration of the environment (35%-70%). An experiment matrix is used that minimizes the number of experiments to be conducted in order to obtain the information needed to meet the scientific objectives.

Because the amount of data to be collected is limited, modeling is necessary to interpret the results and to sort out the important physics of the phenomenon. The modeling effort that will support the experimental program is numerical in nature and includes the capability to solve model flame spread problems over both thermally-thin and thermally-thick fuels posed as steady-state, eigenvalue problems for spread rate or as unsteady momentum, species, and energy equations in the gas and continuity and energy equations in the solid are solved using the SIMPLER algorithm. Gas radiation is included in the model to assist in the interpretation of species-specific emission data obtained with bandpass-filtered video cameras in the experiments.

Task Significance:

Radiative heat and oxygen mass transfer are critical to microgravity fires. In this experiment, very low speed forced flow and radiant heating are imposed on burning samples, and radiant heat loss is measured with state-of-the-art imaging systems. These are the first attempts at such experimental control and measurement in microgravity, and the experimental results and numerical modelling will allow the role of radiation and diffusive transport in these flames to be better understood so that fires in spacecraft can be avoided.

Progress During FY 1996:

The first sounding rocket flight was completed fully successfully in June of 1996. Data analysis is underway, and preliminary results indicate the even a very weak convective flow dramatically accelerates flame spread over thermally-thick solids. A flammability limit for the thick fuel was also found, at much higher oxygen concentration than is found in normal gravity, as theory predicts. Preparations are underway for a second flight in October of 1996.

The mathematical model has been used in parametric studies, and the computational domain, initial conditions, boundary conditions, the solid and gas properties, and ignition power are the same as previously reported. In

previous calculations of the DARTFire matrix, the activation energy of gas phase was 0.89 kJ/kmol. A parametric study was conducted by gradually increasing the activation energy for gas-phase until flame extinction occurs just following ignition.

A 25% increase in activation energy for the 35% O₂ case with the laser on and a flow of 1 cm/s causes the flame to extinguish when the ignitor is turned off, and the drop in temperature is rapid just after the ignitor is switched off. On the other hand, for the 50% O₂ case, a 45% change in activation energy is required to cause extinction, but the extinction takes place 6 to 8 s after the ignitor is turned off. So, it would seem that the 35% case is much closer to extinction than the 50% case and so the fact that in the first flight experiment the case 1 condition extinguished just after ignition is somewhat consistent with what we find here. A 25% perturbation in activation energy is not particularly large.

For 35% with 5 cm/s, a 45% increase in activation energy is needed to cause extinction, the same percentage as in the 50% case. However, the extinction is abrupt as the ignitor is turned off, in contrast to the 6 to 8 s that the flame persists in the 50% environment. Consequently, although it appears that a matrix point of 35% O₂ is somewhat removed from extinction, additional computation and interpretation of the first flight results is needed.

A Web page has been developed to disseminate the DARTFire results through a web browser such as Netscape. The URL is

<http://thermal.sdsu.edu/combustion/dartfire/dartfire.html>

The radiation model is also being compared to two advanced radiation models for source term calculations (the existing model is a global balance (GB) model). In the AI (average intensity) method, the incident radiation at a location is computed to estimate the radiation gain before calculating the source. In the existing method we have no mechanism for calculating any gain. However, the a_p value is still assumed to be a constant. The results from AI method turn out to be almost identical to the GB method, showing not much effect of incident radiation. The source term remains negative throughout the field. In the DT (Discrete Transfer) method, the a_p is varying throughout the field. The contribution from each ray, which may be a net loss or a net gain, to a given control volume is calculated. The results of DT method also agree quite well with the GB method. However, very close to the fuel surface, it shows a slightly positive source term, which is not seen in the other methods.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	0
MS Students:	2	MS Degrees:	2
PhD Students:	2	PhD Degrees:	0

TASK INITIATION: 6/91 **EXPIRATION:** 11/98**PROJECT IDENTIFICATION:** 963-22-05-02**NASA CONTRACT NO.:** NCC3-221**RESPONSIBLE CENTER:** LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Bhattacharjee, S., West, J. and Altenkirch, R.A., "Determination of the spread rate in opposed-flow flame spread over thick solid fuels in the thermal regime." Twenty-Sixth International Symposium on Combustion, The Combustion Institute, August, 1996.

Reflight of the Solid Surface Combustion Experiment with Emphasis on Flame Radiation Near Extinction

PRINCIPAL INVESTIGATOR: Prof. Robert A. Altenkirch

Washington State University

CO-INVESTIGATORS:

Bhattacharjee, S.
Sacksteder, K.R.
Delichatsios, M.

San Diego State University
NASA Lewis Research Center (LeRC)
Factory Mutual Research

Task Objective:

The objective of this flight experiment is to determine the mechanisms of flame spreading over solid fuels in the absence of buoyant or externally imposed, gas-phase flows. This experiment is an extension of the Solid Surface Combustion Experiment with the purpose of observing flame spread with radiative losses near the flammability limit.

Task Description:

The Solid Surface Combustion Experiment (SSCE) is to be reflown to perform additional tests and to obtain quiescent flame spread data for cylindrical, thermally thick fuels. In these tests, measurements of the fuel and flame temperature are to be made and recorded, and the flames will be photographed using motion picture film. The numerical model, developed as part of the SSCE project, is to be further extended to predict flame spread behavior over cylindrical samples in which the geometry of the gas-phase radiative interactions are simplified computationally. A detailed quantitative comparison of the experimental and computational results is to be performed, including comparisons of spread rate, temperature field, heat transfer rates, and flame structure.

Task Significance:

The spreading of flames over solid fuels is a fundamental combustion problem that has practical significance in the prevention and control of fires. Flame spreading in normal gravity is usually dominated by buoyant air flow that introduces a significant complexity into fundamental theoretical models. Experiments conducted in the microgravity environment nearly eliminate this complexity, providing a more fundamental scenario for the development of flame spreading theory.

Progress During FY 1996:

1) A Microgravity Hardware Reflight Review (MHRR) was held to peer-review the science requirements for the reflight of the Solid Surface Combustion Experiment and to determine the hardware readiness for these missions. The MHRR was concluded successfully, with the authority to proceed with the hardware preparations for two additional Shuttle flights.

The approved flight tests consist of:

A. Near Limit Flat Sample: The first reflight test will be similar to the last three tests of the original SSCE tests using flat PMMA samples. In this case however, a single sample will be burned that is twice as long as the previous sample pairs. The objective will be to try to observe the entire history of the spreading from ignition to a quenching that is predicted to occur by the numerical model. The test condition will be 50% oxygen/50% nitrogen at one atmosphere of pressure.

B. Cylindrical Samples: The second reflight test will take advantage of the comparative simplicity of the cylindrical geometry for radiative heat transfer calculations. Two samples will be burned: the first will be a small diameter (3mm) which is predicted to burn steadily because of its small thickness. The second will be a larger diameter cylinder with both a hollow and a solid section. The larger diameter hollow section is predicted to burn steadily while the solid section should exhibit unsteady burning behavior.

2) Additional 5.2 second drop tower tests were conducted to confirm the test conditions for the near extinction flight test and the ignition behavior of the cylindrical samples for the second flight test. The flat samples seem to be unignitable in the available test time at atmospheric conditions of 40% oxygen/60% nitrogen at 1 atmosphere, but

are clearly ignitable in 50% oxygen at the same pressure. The flight design of the cylindrical samples were tested, including the ignitor wire path configurations and sample mounting schemes.

3) At the end of the year potential flight assignments were under study, the first of which is STS-86 in the summer of 1997.

FY 96 Publications and Presentations are listed under the original SSCE program entitled, "Scientific Support for an Orbiter Middeck Experiment on Solid Surface Combustion."

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 4
PhD Students: 1

TASK INITIATION: 5/94 EXPIRATION: 11/97

PROJECT IDENTIFICATION: 963-15-0E

NASA CONTRACT No.: NCC3-354

RESPONSIBLE CENTER: LeRC

Gravitational Effects On Laminar, Transitional, and Turbulent Gas-Jet Diffusion Flames

PRINCIPAL INVESTIGATOR: Dr. M. Y. Bahadori

Science Applications International Corporation

CO-INVESTIGATORS:

Hegde, U.G.

NYMA, Inc.

Task Objective:

The overall objective of this program is to improve our fundamental understanding of microgravity gas jet diffusion flames in the entire laminar, transitional, and turbulent regimes. Specifically, tests are to be conducted in microgravity with the purpose of (i) determining the effects of buoyancy on these flames, (ii) determining the relative importance of buoyancy-induced turbulence on flame characteristics, (iii) revealing phenomena which may be masked by buoyant convection, and (iv) characterizing the processes of vortex/flame interaction for a better understanding of transition to turbulence of gas jet diffusion flames.

Task Description:

In order to achieve these objectives, the program pursues two distinct but complementary paths, as follows:

(a) Investigating the effects of fuel type, flow rate, Reynolds number, nozzle size, and gravity on (i) global flame characteristics (such as flame shape, height, radiation and temperature), (ii) the extent of the transition regime, (iii) turbulent flame features, and (iv) stand-off characteristics and blow-off conditions. These tests provide data on flames in microgravity (using the Drop Tower and Zero-Gravity Facility, in addition to the KC-135 aircraft) and normal-gravity environments. The measurements include temperature, thermal radiation, pressure, species concentration, acceleration, and flame imaging. The data will be used to validate detailed analytical and numerical models of these flames.

(b) Identifying the mechanisms involved in the generation and interaction of observed large-scale structures which directly influence the flame characteristics noted under (a). This part involves an investigation to be carried out in space, which utilizes a controlled, well-defined set of disturbances to reveal the mechanisms that govern the dynamics of large-scale structures interacting with flame fronts under microgravity conditions. This will further our understanding of the naturally occurring disturbances that are an inherent part of the transitional and turbulent flames of part (a). As in part (a), a combined analytical and numerical modeling effort will be an integral component of this phase of the program.

Task Significance:

Most practical combustion is turbulent because enhanced mixing is essential for increasing combustion efficiency. Despite this technical importance, turbulent flames are not well understood because their random, transient nature greatly complicates the interaction of processes occurring in flames and their associated analysis. This complication is overcome in a microgravity experiment through the use of a steady laminar flame and induced vortices. Controlled, repeating vortices are produced by an iris mechanism that opens and partially closes around the base of the flame. The operation of the mechanism creates sinusoidal variations in the air flow entrained by the fuel jet, at a single controlled frequency. The experiment cannot be conducted in normal-gravity because buoyant instabilities induce uncontrolled vortices at other frequencies and amplitudes, complicating the analysis. The results of this experiment will help in improving our understanding of turbulent flames with direct applications to problems of combustor efficiency and pollutant emission.

Progress During FY 1996:

Contract NAS3-25982 has been in place since November 1991. It involves a comprehensive study of laminar, transitional, and turbulent gas jet diffusion flames in microgravity. The following researchers participated in this effort: 1) M.Y. Bahadori, Principal Investigator (SAIC); 2) U.G. Hegde, Co-Investigator (NYMA, Inc.); 3) D.P. Stocker Project Scientist (NASA Lewis); and 4) F. Vergili, Project Manager (NASA Lewis).

Fabrication of the flight experiment package is near completion. Testing and verification are underway, and the integration/payload preparation phases are scheduled for late 1996. To-date, the fuel system is in place, video

cameras and mirrors are mounted, PCU assembly is done, and DACS board is completed. In addition, the ignition algorithm for flight experiment is finalized, and verification matrix for the hardware is prepared. The verification/system review was successfully held. Calculations were performed for the worst-case products analysis, and for the explosion safety analysis. The field of view of the radiometers and the time constant of the flight thermocouple rake were measured. Vibration testing of the color camera and thermocouples were successful. Other tests included synchronization of the fuel flow and ignitor heat up, flight ignitor test, chamber hydraulic test, and leak testing of the fuel assembly system and solenoid valves. In addition, the VTR, IPU, and color camera successfully passed the thermal cycling test.

A number of documents were prepared following the component testing and hardware fabrication processes. These include: (a) procedure and analysis document for the explosion test; (b) products analysis document; (c) safety data package; (d) contamination control document; (e) radiometer characterization report; (f) payload accommodation requirements document; (g) software requirements and preliminary design document; and (h) products assurance plan.

More than twenty-five tests were conducted in the Zero-Gravity Facility for iris verification, flame characterization, thermocouple-rake operation, global radiometer performance, slice radiometers measurements, and visualization characteristics. In addition to the flight test matrix of the pulsed gas jet diffusion flame, different iris frequencies, thermocouple locations, radiometer locations, iris settings, (limited) environmental conditions of pressure and oxygen concentration, and fuel flow rates were utilized to better characterize the matrix for the flight experiment. These tests have resulted in important findings regarding the characteristics and structure of jet diffusion flames under the influence of imposed pulsations with well-defined, controlled parameters. The results are presented in a number of publications, which are shown in the bibliography.

The radiation data have shown the importance of radiometer location for maximum signal, which is different for normal-gravity and microgravity flames. Theoretical modeling used in this program has confirmed this finding. It was also found that temperature oscillations have a decreasing amplitude downstream of the microgravity flame, which is in contrast to behavior in normal gravity regarding the decay in temperature dissipation. In addition, significant characteristics of vortex/flame interactions in microgravity flames have been observed, which include the near-unity coherence, temperature and radiation response to the frequency of imposed oscillations, and phase relations of flame properties. Data from measurements on flame oscillation under different gravitational levels were analyzed and compared with the results from numerical modeling. The agreement is excellent, and the results establish correlations for flame flicker frequency as a function of gravity level, in addition to providing relationships for dependence of velocity on both axial distance and gravitational level.

Numerical and analytical modeling are currently in progress for simulation of the vortex/flame interaction process in microgravity. The predicted velocity and temperature fields under the influence of iris-induced flow have shown the phase differences resulting from the effect of vortex dynamics, dissipation decay along the flame, sinusoidal variations of local velocity and temperature, and flame front oscillation in the presence of moving vortices. The oscillatory temperature behavior has been verified by comparison with experimental results, and phase differences at different locations both inside and outside the flame have been confirmed. The computational results from the transient numerical model also provided the optimum number of iterations for simulation of the pulsed microgravity flame. This has not only facilitated the calculations for iris pulsations over many cycles, but has also reduced the computational time by more than 50%. It has also shown that residuals of the variables, such as velocities, are orders of magnitude smaller than the initial residuals, which makes the iteration results quite accurate. In order to obtain a dynamically stable mode in predictions, simulations were performed for a number of consecutive iris cycles, and the results were compared for differences between these cycles. The error in the field parameters during the final cycles of the iris was extremely small, indicating that dynamic stability in the predictions was obtained. The modeling work is in progress for comparisons of predictions with the data.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 0

TASK INITIATION: 11/91 **EXPIRATION:** 12/98**PROJECT IDENTIFICATION:** 963-22-05-03**NASA CONTRACT NO.:** NAS3-259**RESPONSIBLE CENTER:** LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Hegde, U., Zhou, L., and Bahadori, M.Y., Winner of the SAIC 1995 Publications Prize in Physics: "The transition to turbulence of microgravity gas jet diffusion flames". Combustion Science and Technology, vol. 102, no. 1-6, pp. 95, 1994 (November 1996).

Proceedings

Bahadori, M.Y., Small, J.F., Hegde, U., and Stocker, D.P., "Single-point measurements and predictions of radiative loss from buoyant and non-buoyant jet diffusion flames." Proceedings of the Central States Meeting of The Combustion Institute, St. Louis, MO, May 1996.

Bahadori, M.Y., Small, J.F., Hegde, U., and Stocker, D.P., "Measurements and predictions of the temperature field of a microgravity diffusion flame." Proceedings of the Western States Meeting of The Combustion Institute, Los Angeles, CA, October 1996.

Bahadori, M.Y., Zhou, L., Stocker, D.P., and Hegde, U., "Measurements of flame flicker under different gravitational levels." Proceedings of the Fall Eastern States Meeting of The Combustion Institute, Hilton Head, SC, 1996.

Hegde, U., et al., "Microgravity environment and its effects on science." Proceedings of the AIAA-96-0401, Invited Panel Presentation at the AIAA 34th Aerospace Sciences Meeting, Reno, NV, January 1996.

Hegde, U., Stocker, D.P., and Bahadori, M.Y., "Temperature correlations in a pulsed microgravity diffusion flame." Proceedings of the AIAA-96-0261, AIAA 34th Aerospace Sciences Meeting, Reno, NV, January 1996.

Hegde, U., Stocker, D.P., and Bahadori, M.Y., "Unsteady diffusion flames in microgravity." Proceedings of the Fall Eastern States Meeting of The Combustion Institute, Hilton Head, SC, 1996.

Presentations

Bahadori, M.Y., "Laminar, transitional, and turbulent jet diffusion flames in microgravity." Center for Energy and Combustion Science, University of California, San Diego, October 1996.

Sooting and Radiation Effects in Droplet Combustion (SEDC)

PRINCIPAL INVESTIGATOR: Prof. Mun Y. Choi

University of Illinois, Chicago

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

To determine the effects of sooting on droplet combustion characteristics using optical and intrusive techniques. The parameters to be studied include burning rate, flame dynamics, extinction, disruption and soot particle dynamics.

Task Description:

The sooting behavior will be studied using expanded beam line-of sight extinction and subsequent 3-point Abel deconvolution to determine the soot volume fraction distribution; two-wavelength optical pyrometry to determine the soot temperature within the region between the flame and the droplet; and thermophoretic sampling/transmission electron microscopy to determine the soot morphology (radius of gyration, primary particle size, fractal geometry, etc). Feasibility studies will also be performed using Laser-Induced-Incandescence techniques to determine droplet soot volume fraction.

These experiments will be performed for a wide range of conditions to vary the sooting propensity of the droplet using various fuels, pressure, oxygen indices, droplet dimension and inerts as parameters. In addition, computational modeling of the soot particle dynamics using the balance between thermophoresis and Stefan drag will be compared with the experimental measurements. The modeling efforts will be advanced interactively with the experimental measurements of the soot volume fractions and the soot particle dimensions.

Task Significance:

The combustion of a pure, single-component liquid droplet provides an ideal problem from which to obtain valuable information for both basic and applied scientific purposes. The importance of the isolated droplet burning process has promoted extensive experimental and theoretical investigations for more than 40 years. In terms of the practical relevance, the knowledge of individual droplet burning characteristics provides insights into some of the more complex mechanisms involved in spray combustion. Since estimated energy production through spray combustion processes accounts for more than 25% of the world's output, droplet combustion remains a viable field for continued research.

Since the pioneering microgravity droplet combustion experiments of Kumagai and coworkers back in 1957, there have been numerous theoretical, computational and experimental studies analyzing the burning characteristics of isolated droplets. However, sooting effects have typically been neglected due to the complexities involved (both experimental and computational/theoretical). However, recent microgravity experiments indicate that soot/sootshell formation affects all four of the important measurable parameters involved in droplet combustion: burning rate, flame diameter, extinction and disruption. Thus, our understanding of the burning characteristics of droplets can only be complete by considering a detailed study of the sooting behavior for a wide range of characteristic times and dimensions.

In all previous microgravity studies, the degree of sooting was estimated by visual observations of the sootshell. This study will focus on the effects of sooting on the droplet burning rate, flame dimensions, extinction and disruption by accurately measuring the soot volume fraction, temperature and soot morphology and dynamics. These measurement of the temperature and soot volume fractions will also prove beneficial in assessing the importance of radiative heat transfer.

Progress During FY 1996:

In the last year, we concentrated our efforts on performing tests with the experiment hardware in the 2.2 Second Drop Tower at NASA LeRC. The experiment hardware consists of a combustion chamber within which is a droplet deployment and ignition system (based on the Droplet Combustion Experiment design). Several windows in the

chamber provide optical access. A laser back-lit image of the droplet region enables the quantitative determination of the soot volume fraction in the gas-phase, a back-lit image of the droplet alone provides a measure of the droplet burning rate, and two additional video cameras and filters enable determination of the gas-phase temperature field using two-wavelength optical pyrometry. Finally, a thermophoretic soot sampling probe allows us to gather soot samples for subsequent analysis using an electron microscope.

In the first test series, single droplets of heptane or decane (pure hydrocarbon fuels, common components of practical fuels) were suspended on a 15 micron diameter silica carbide fiber. These droplets were ignited by a hot-wire in microgravity, and the resulting flame and soot development was recorded.

In these initial tests, considerable fine-tuning of the soot volume fraction optics was needed. A vibration problem (associated with the release of the experiment hardware into free-fall) was isolated, and the component shift reduced to 0.2 mm. In addition, the ideal choice of neutral density filter was determined. The goal was to choose it such that enough of the laser light passed through while cutting off flame radiation. Finally, a procedure yielding accurate background intensity information was established (important for quantifying the soot volume fraction).

A total of 96 drops were conducted of which 46 were successfully ignited, and ten of these produced nearly-spherical soot shells. The time-varying soot distributions within the region bounded by the droplet surface and the flame were measured using the full field light extinction technique and subsequent tomographic inversion using Abel transforms. For the first time ever, a quantitative assessment of the degree of sooting for isolated droplets burning under microgravity conditions was obtained using n-heptane as the fuel. (Decane tests always produced optically thick sooting regions.)

Testing was temporarily suspended for four months after a failure of the experiment deceleration system at the drop tower which severely damaged the experimental apparatus. Almost all of the electrical components, the chamber, and its contents survived, but most mechanical parts and structures outside of the chamber were damaged. The thermoelectric cooler for the laser was returned to the manufacturer for repair. NASA engineers and technicians rebuilt the rig, and all the optical components were reinstalled and calibrated. During this rebuild phase, the thermophoretic soot sampler was incorporated into the hardware.

In the second test series, the rebuilt rig worked flawlessly and more than 80 drops were performed using heptane as the fuel. Of these, 22 tests yielded spherical or nearly-spherical soot shells. The initial droplet diameter was varied from 0.8 to 1.8 mm and the ambient pressure from 0.5 to 1.0 atm. The thermophoretic soot sampler was used to obtain soot samples from microgravity droplet flames for the first time.

Drop tower results enable the following conclusions to be made about microgravity droplet combustion.

- 1.) Soot production is more concentrated in microgravity compared to normal gravity (some cases as high as 60 ppm volume fraction compared to 1 ppm). The absence of buoyancy allows the thermophoretic force to become important, permitting a 'soot cloud' to build up between the droplet surface and the flame.
- 2.) While the distribution of soot volume fraction is similar for different initial droplet diameters (for the observation times available) the total mass of soot contained by the flame is substantially larger for the larger droplets. This effect is expected to become even more dramatic given longer observation times.
- 3.) Droplets of heptane yielded lower soot concentrations at reduced pressure.
- 4.) Examination of the soot samples using an electron microscope showed that the soot is much different when formed in microgravity, as seen in other diffusion flame configurations.

After these drop tower tests, the experiment hardware was reconfigured and loaded onto the NASA LeRC DC-9 reduced gravity aircraft for access to a longer-duration microgravity. Since we always intended to perform tests on the DC-9, the reconfiguration was very easy. The main task was simply mounting the experiment hardware and support equipment inside the aircraft. The support equipment consisted of three VCR's, a monitor, a pump, gas bottles for filling the chamber, and a control box.

In this first aircraft test campaign, heptane droplets in air at normal pressure were burned. The initial droplet size was varied up to 5 mm diameter. The experiment hardware was always bolted to the aircraft (no 'free-float' tests were performed) so that the droplets and flames experienced g-jitter (vibration associated with the aircraft maneuvers).

The following conclusions are drawn from the aircraft tests:

- 1.) Stabilization and ignition of large droplets with the current system is possible.
- 2.) The soot cloud and flame structure are greatly disturbed by g-jitter.
- 3.) Thermophoretic soot samples for large initial droplet diameters were obtained.

Along with these microgravity drop tower and aircraft tests, normal-gravity tests were performed in parallel, yielding some interesting results. The non-intrusive, full-field, optical soot volume fraction technique, described above, was compared to gravimetrically measured soot content for various droplet flames burning in normal gravity and at reduced pressure. (The gravimetric technique relies on carefully weighing the soot produced for a given droplet. It is a macroscopic measure of soot production.)

The optical measurements provide the temporally and spatially resolved structure of the sooting region within the flame. Results indicate that the maximum soot volume fraction along each vertical location above the droplet decreases linearly with reduction in ambient pressure. However, this trend cannot be explained solely by changes in the adiabatic flame temperatures (caused by pressure reductions). The more important reasons are the changing flow configuration and shorter residence time for fuel pyrolysis and reactions leading to soot formation.

Gravimetrically-collected soot emitted through the open tip flame displays the same linear variation with pressure as maximum soot volume fraction. As a result, the soot conversion ratio and soot yield can be evaluated using the calibrated maximum soot volume fraction. Therefore, with the non-intrusive optical measurements, it is possible to determine both the detailed structure of the sooting region within the flame (important to characterize the radiative characteristics of the flames) as well as the total soot that is emitted to the environment. In addition, the soot threshold pressure, below which no soot is formed, is determined by extrapolation.

In other normal-gravity work, the two-wavelength pyrometry technique was calibrated by using the well-characterized 'Santoro' burner as a benchmark. The gas phase temperature field for this burner is known, so the output from the pyrometry cameras could be properly interpreted to yield the temperature field for unknown distributions.

In the modeling effort, the PI arranged for collaboration with Professor Frederick Dryer of Princeton University using an empirical soot formation/growth mechanism in the Chemically Reacting Flow Model. The experimental results will be used to determine the correct parameters for the soot model. In turn, the model will calculate the effect of soot on flame temperature, burning rate, flame structure, and kinetic extinction behavior.

The Science Concept Review is scheduled for early FY97. In preparing for this review the first draft of the Science Requirements Document was completed. Additionally, we presented an overview of our experiment requirements to the Space Station Fluids and Combustion Facility project team as a potential basis combustion experiment for the facility.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 3

TASK INITIATION: 6/94 EXPIRATION: 5/98

PROJECT IDENTIFICATION: 963-15-0B

NASA CONTRACT NO.: NAG3-163

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Choi, M.Y. and Lee, K.-O., "Investigation of sooting in microgravity droplet combustion." Proceedings of the Central States Section Meeting of the Combustion Institute, St. Louis, MO, May, 1996.

Presentations

Choi, M.Y. and Lee, K.-O., "Investigation of sooting in microgravity droplet combustion." 26th Symposium (International) on Combustion, The Combustion Institute, 1996.

Lee, K.-O., Jensen, K.A., and Choi, M.Y., "Investigation of sooting in normal-gravity droplet combustion using light extinction and gravimetric techniques." Twenty-Sixth International Symposium on Combustion, The Combustion Institute, 1996.

Lee, Kyeong-Ook, Jensen, K.A., Choi, M.Y., "Measurement of soot volume fraction of single droplets using light extinction technique." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28-August 2, 1996.

Candle Flames in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Daniel L. Dietrich

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

Ross, H.D.

Tien, J.S.

NASA Lewis Research Center (LeRC)
Case Western Reserve University**Task Objective:**

The goal of this work is to further investigate some of the features of candle flame combustion observed during a recent small scale candle flame experiment conducted on board the space shuttle. These are specifically as follows:

1. To observe whether a steady flame can exist in a purely diffusive environment;
2. To understand from a fundamental aspect the observed near-extinction flame oscillations;
3. To examine the nature of the interactions between two candle flames.

As a secondary objective, we will use the candle as a model system (non-propagating, steady-state diffusion (non-convective) flame) to investigate buoyant scaling arguments for diffusion flames. Testing and scaling analysis to date shows that utilizing reduced pressure, enhanced oxygen environments do not produce a buoyancy-free environment, as currently published scaling arguments suggest.

Task Description:

These objectives will be accomplished by a program consisting of the development of a comprehensive numerical model of the candle flame, ground-based testing in normal-gravity laboratories and drop towers, and another small-scale glovebox experiment.

The development of a comprehensive numerical model represents the most significant addition to the proposed program. The gas-phase model will be a modification of an existing two-dimensional code developed for flame spread over solid fuels under the guidance of one of the investigators. The initial model for the wick/liquid phase has already been developed by the principal investigator.

The ground based testing will utilize existing drop rigs and other existing experimental equipment to fully characterize the candle flame in a range of ambient conditions (i.e., atmospheric to sub-atmospheric pressures, nitrogen-oxygen, helium-oxygen ambients). The data will be imaging of the flame, thermocouple measurements, LDV and possibly PIV, all of which the investigators have experience using. The use of more advanced diagnostics will also be explored during the later phases of the program.

The space experiment will be a glovebox experiment that is similar to the existing Candle Flame in Microgravity glovebox experiment (same investigators). The minor proposed changes will be: a larger free volume, the performance of the thermocouple measurements (a capability that existed but was not used on the last experiment because scheduling conflicts), the ability to maintain a large candle separation distance and to simultaneously ignite the two candles.

Task Significance:

The candle flame in microgravity is a unique/model system (non-propagating, steady-state diffusion (non-convective) flame). The data from this work is expected to improve our understanding of diffusion flames on a fundamental level.

Progress During FY 1996:

Experimental

The candle flames project was flown as a MIR glovebox experiment. This experiment was an enhancement of the USML-1 experiment with the following features: 1) a larger candle box with a greater free area which should translate into a longer flame lifetime, 2) more candles to develop statistics of the combustion process, 3) temperature measurements using fine wire thermocouples, 4) point measurements of the flame luminosity, 5) point measurements of the far-field oxygen concentration, 6) automatic ignition and simultaneous ignition of two candles, and 7) candles with different wick diameters and lengths and different candle diameters. Astronaut Dr. Shannon Lucid began CFM operations aboard Mir on July 1, 1996. Data from this experiment to date suggest long-term flame survivability and showed evidence of spontaneous, and prolonged flame oscillations near extinction. Testing on Mir was completed on July 26, 1996. All of the data (video, temperature, oxygen, and radiometric) will be returned on the STS-79 mission.

Modeling

Because of the large domain of influence from a spherical flame in zero gravity and the need to place fine grids near the reaction zone, the cylindrical coordinates system originally used in the research was abandoned. Instead, a spherical coordinate system has been adopted. Considerable effort has been spent to formulate the problem in the new coordinate system using the control volume approach. Although the formulation is two-dimensional (i.e., two independent variables), the initial test is for a one-dimensional calculation using a two-dimensional code is that we know how the 1-D flame behaves, so it is a good test case. Several test results appeared to be successful, but one test case was found to have an inconsistency. The cause of the problem is currently being investigated.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 1
PhD Students: 0

TASK INITIATION: 5/94 EXPIRATION: 4/98

PROJECT IDENTIFICATION: 963-15-0B

RESPONSIBLE CENTER: LeRC

Investigation of Laminar Jet Diffusion Flames in Microgravity: A Paradigm for Soot Processes in Turbulent Flames

PRINCIPAL INVESTIGATOR: Prof. Gerard M. Faeth

University of Michigan

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The flight project is an experimental and theoretical investigation of the mechanisms of soot formation in laminar jet diffusion flames under conditions of low buoyancy. The flight experiment is in the Combustion Experiment Module.

Task Description:

Several types of experiments have been conducted. The majority have been in normal gravity, studying the influence of gravity by varying the ambient pressure. In addition, experiments have been conducted on NASA's low gravity aircraft, (the KC-135 at JSC). The work has focused on mapping soot volume fraction, temperature, soot particle size and gas species in a variety of hydrocarbon flames. The flight experiment will be limited to measurement of soot volume fraction, soot particle size and some temperatures.

Task Significance:

In most flames of practical interest, soot radiation is the dominant mode of heat transport to combustor components and a dominant mechanism for flame spread and growth. The experimental results, combined with theoretical modelling will confirm or deny the applicability of the conserved scalar formalism to soot properties in diffusion flames. These results, when combined with those of ground-based low- and normal gravity experiments will increase the current fundamental understanding of soot formation processes in both laminar and turbulent flames and increase our ability to model them. Consequently this will have a significant impact on our understanding of systems such as the spread of unwanted fires, design of jet engines and large scale boilers.

Progress During FY 1996:

Subject: Cumulative report for Laminar Soot Processes (LSP), FY95

1 October

1995 - 30 September 1996

Laminar Soot Processes (LSP)

October

Measurements of the concentration of stable gas species of intermediate flames were completed; predictions also were prepared for these results finding excellent agreement between measurements and predictions using either the Leung & Lindstedt or Frenklach et al. mechanisms. Calculations of soot growth rates in our flames were also found to be in good agreement with the HACA mechanism of Frenklach et al.; thus, loss of surface reactivity with streamwise distance is due to reduced H atom concentrations, not age as thought by some earlier workers. These findings are being summarized in a paper while new test conditions to highlight trends of soot processes are being selected; this work will continue throughout the next report period. Interactions with NASA - LeRC about LSP and write-up of experimental procedures will continue as well.

November

Measurements of the concentrations of stable gas species were repeated successfully for all the flames. All results have been tabulated and plotted as part of preparation of a paper which describes these results. Current work involves checking all calculations of soot growth rates, evaluation of predictions of gas compositions for other experimental conditions reported in the literature, and selecting new conditions to test the HACA mechanism. Interactions with NASA-LeRC about LSP include setting up equipment to test the laser extinction and multiline emission measurements, and write-up of test procedures; this work will continue throughout the next report period as well.

December

Predictions of yields of major gas species and hydrocarbons were evaluated for the methane/oxygen flames of Ramer et al. finding good agreement using either the Leung & Lindstedt and the Frenklach et al. mechanisms. A general plot of the HACA soot growth mechanism was carried out using our measurements; encouraging correlation between measurements and predictions was obtained for a reasonable collision efficiency of 1/25, supporting our earlier findings. Evaluation of the HACA soot growth mechanism highlighted the value of the test conditions of Ramer et al.; therefore, measurements for these conditions have been initiated and will continue for the next few report periods. Interactions with NASA-LeRC about LSP continued.

January

Calculations were carried out which show that H atom concentrations are in equilibrium in our premixed flames; therefore, we are modifying our data reduction so that our estimates of H come from this assumption and our measurements of hydrogen concentrations and temperatures. We carried out a quantitative comparison between our growth measurements and the HACA mechanism of Frenklach and coworkers; the results are promising but recent extensions have the potential for significant improvements so we are examining them. Apparatus development and tests continued for premixed and (LSP) diffusion flames, and will continue for the next report period.

February

All premixed flame measurements were corrected to use our new estimates of H atom concentrations based on the assumption of thermodynamic equilibrium. We completed a quantitative comparison between our growth measurements in premixed flames and the predictions of the HACA mechanisms of Frenklach and coworkers and Colket and Hall; the latter yields an excellent correlation and these evaluations have now been reported in a paper by Xu et al. submitted to Combustion and Flame. Analogous work is in progress for our earlier growth measurements in diffusion flames; this work will continue throughout the next report period. Test conditions for new measurements of soot processes in premixed flames have been established to compliment our earlier measurements; these experiments will continue for the next several report periods. Apparatus development continued for the LSP diffusion flames, and will continue for the next report period.

March

We continued evaluation of the HACA mechanisms based on our earlier measurements in diffusion flames. The results are very promising and indicate reasonable levels of H atom super equilibrium in the soot formation regions; we now are studying ways to quantify these super equilibrium levels. Measurements have begun for the new test conditions established for premixed methane/oxygen flames; these measurements will continue for the next few report periods. Apparatus development continued for the LSP diffusion flames with completion and satisfactory evaluation of burner operation; instrument assembly will be undertaken during the next report period.

April

Three fuel-rich soot-containing laminar premixed methane/oxygen flames have been established for various C/O ratios and tests to measure soot and flame structure in them have been initiated. Measurements of soot concentrations have been completed by deconvoluting laser extinction measurements for cord-like paths. Current work involves multiline emission measurements to find soot temperatures; this work will continue throughout the next report period. Our recent evaluation of the HACA soot growth mechanism of Frenklach and coworkers for laminar premixed ethylene/air flames is being extended to include recent results by these authors to correlate their imperial stearic factor as a function of temperature; this work will continue throughout the next report period. Finally, apparatus development for the LSP diffusion flames, establishing two test diffusion flames and measuring their radiative heat loss fractions, was completed satisfactorily. Current work involves laser extinction measurements of the LSP flames; this work will continue throughout the next report period.

May

Multiline emission measurements to find soot temperature distributions in the three fuel-rich soot-containing laminar premixed methane/oxygen flames are nearing completion; other measurements in these flames will continue throughout the next report period. The recorrelation of the stearic factor as a function of temperature for the HACA soot growth mechanism of Frenklach and coworkers was completed; revision of the paper describing these results should be completed during the next report period. Finally, laser extinction measurements were completed for the LSP flames; current work involves the laminar smoke point properties of butadiene and propylene/nitrogen flames, this work will continue throughout the next report period.

June

Multiline emission measurements of soot temperatures were completed for all three fuel-rich soot-containing laminar premixed methane/oxygen flames; additional checks of results at a few conditions should be completed early in the next report period. Subsequent work will involve soot structure and near-burner thermocouple temperature measurements. Revision of the paper describing the earlier premixed flame measurements is still in progress but should be completed during the next report period. Measurements of laminar smoke point properties of butadiene-and propylene-nitrogen mixtures were completed. For reference purposes, similar measurements are being carried out for ethylene-and propane-nitrogen mixtures; this work should be completed during the next report period.

July

Multiline emission measurements of soot temperatures were checked satisfactorily for all three fuel-rich soot-containing laminar premixed methane/oxygen flames. Current measurements for these flames involve near-burner temperature measurements with fine-wire thermocouples corrected for radiative heat losses; these measurements will continue throughout the next report period. The paper describing the earlier premixed flame measurements has been revised and resubmitted. Measurements of the laminar smoke point properties of fuel/nitrogen mixtures of the test fuels have been completed and butadiene/nitrogen and propylene/nitrogen flames have been selected that have the same laminar smoke point flame lengths as ethylene; current work involves traversing measurements of soot concentrations and temperatures of 35 and 70 mm long flames of these two reactants.

August

Measurements of near-burner temperature distributions using fine-wire thermocouples corrected for radiative heat losses were completed satisfactorily; measurements of species concentrations have begun and will continue throughout the next report period. Traversing measurements of normal gravity flames of ethylene, propane, propylene/nitrogen and butadiene/nitrogen flames have been completed to find soot volume fraction distributions; multiline temperature measurements for these flames are in progress and will continue throughout the next report period.

September

Species concentration measurements were initiated for the test flames. Corresponding computations were initiated as well with initial results found to be quite promising. Multiline temperature measurements were completed for the normal gravity flames and corresponding corrected thermocouple measurements were initiated for the soot-free portions of these flames. All these activities will continue throughout the next report period.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 2/91 EXPIRATION: 2/01

PROJECT IDENTIFICATION: 963-22-05-04

NASA CONTRACT NO.: NAG3-124

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Faeth, G.M. and Koylu, U.O., Soot morphology and optical properties in nonpremixed turbulent flame environments. *Combust. Sci. Tech.*, vol. 108, no. 4-6, pp. 207-229 (October, 1995).

Koylu, U.O. and Faeth, G.M., Spectral extinction coefficients of soot aggregates from turbulent diffusion flames. *J. Heat Trans.*, vol. 118, no. 2, pp. 415-421 (1996).

Koylu, U.O. and Faeth, G.M., Spectral extinction coefficients of soot aggregates from turbulent diffusion flames. *J. Heat Trans.*, vol. 118, no. 2, pp. 415-421 (1996).

Lin, K.-C. and Faeth, G.M., Effects of hydrodynamics on soot formation in laminar opposed-jet diffusion flames. *J. Prop. Power*, vol. 12, no. 4, pp. 691-698 (1996).

Lin, K.-C., Sunderland, P.B., and Faeth, G.M., Soot nucleation and growth in acetylene/air laminar coflowing jet diffusion flames. *Combust. Flame*, vol. 104, no. 3, pp. 369-375 (1996).

Xu, F., Sunderland, P.B. and Faeth, G.M., Soot formation in laminar premixed ethylene/air flames at atmospheric pressure. Combustion and Flame, (In press 1996).

Proceedings

Faeth, G.M., and Koylu, U.O., "Structure and optical properties of flame-generated soot." Proceedings of the 8th International Symposium on Transport Phenomena in Combustion, Taylor and Francis New York, September 1996.

Koylu, U.O. and Faeth, G.M., "Spectral extinction coefficients of soot aggregates from turbulent diffusion flames." Proceedings of the Fall Technical Meeting, Eastern Section of the Combustion Institute, Pittsburgh, PA, pp. 211-214, October 1995.

Lin, K.-C. and Faeth, G.M., "Effects of hydrodynamics on soot formation in hydrocarbon-fueled laminar opposed jet diffusion flames." Proceedings of the Fall Technical Meeting, Eastern Section of the Combustion Institute, Pittsburgh, P.A. pp.423-426, October 1995.

Lin, K.-C. and Faeth, G.M., "Structure of laminar permanently-blue opposed-jet hydrocarbon fueled diffusion flames." Proceedings of Spring Technical Meeting, Central States Section, The Combustion Institute, Pittsburgh, pp. 110-115, May 1996.

Presentations

Faeth, G.M., "Laminar Soot Process (LSP) experiment." MSL-1: Third IWG Meeting, Marshall Space Flight Center, Huntsville, March 1996.

Lin, K.-C., "Soot control in laminar opposed-jet diffusion flames." Fluid and Gas Dynamics Seminar, Department of Aerospace Engineering, The University of Michigan, October 1995.

Xu, F., "Soot nucleation and growth in laminar premixed flames." Fluid and Gas Dynamics Seminar, Department of Aerospace Engineering, The University of Michigan, November 1995.

Xu, F., Sunderland, P.B., and Faeth, G.M. "Measurements and predictions of soot formation in laminar premixed flames." Proceedings of Spring Technical Meeting, Central States Section, The Combustion Institute, Pittsburgh, May 1996.

Unsteady Diffusion Flames: Ignition, Travel, and Burnout

PRINCIPAL INVESTIGATOR: Dr. Frank Fendell

TRW

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Investigate the adequacy of frequently adopted, simplified mathematical models to describe the behavior of laminar flames, primarily diffusion flames, by comparison with definitive experimental data, conveniently available from burning in a microgravity environment.

Task Description:

A combined experimental and theoretical approach is used, in which a stable, planar, virtually strain-rate-free diffusion flame is achieved by experimental design. The high degree of spatial symmetry is a simplification for both data collection and modeling. Parametric variation of initial stoichiometric proportion and reactant dilution is to provide sufficient data to test models.

Task Significance:

The adequacy of frequently used models to predict diffusion-flame behavior can be tested. This project will facilitate comparison of the accuracy of alternative diffusion-flame models, from the relatively simple to the highly inclusive. Clarifying what minimal level of inclusiveness in formulation suffices to meet a user's requirements is practically advantageous. The work is particularly pertinent for flames with gaseous fuels, such as hydrogen, natural gas and propane, and near-cold-wall quench layers. The approach may be extended for the study of other gaseous chemically reacting systems.

Progress During FY 1996:

The effective starting date of the contract NAS3-27264 is July 11, 1994. LeRC and TRW have agreed on revisions to the contract based on the mutually agreed planned activities of TRW during the second year of the contract. The planned activities for TRW for the second year were not compatible with the original Statement of Work of the contract. The official amendment for the modification to the contract is signed by the respective Contracting Officers effective October 3, 1995.

The plan is to initially segregate hydrogen diluted with argon, and oxygen diluted with helium, into two equal half-volumes within a squat rectangular-solid-configured container with isothermal, noncatalytic, impervious walls. The contents of the two half volumes are each to be at atmospheric pressure and temperature, and to have equal density, so that the "average molecular weight" for each half volume is the same. The overall contents are to be sufficiently fuel-deficient such that, if (conceptually) the initial, segregated contents of the container were mixed to form a perfectly homogeneous gaseous mixture, the adiabatic flame temperature (equilibrium burned-gas temperature) would be consistent with a vigorous diffusion flame, but not so hot that either dissociation of product species (mainly water vapor) or gaseous radiative heat transfer or the physical integrity of the container is of concern.

In practice, a thin metallic film is to serve as the impervious initial interface between the half volumes; it is to be removed, on command, by rapid lateral translation in its own plane. Ignition, probably by spark, is to occur after very a short interval for reactant interdiffusion. Aside from possible exceptions at early times, the diffusion flame is anticipated to travel into the hydrogen-containing half volume. The key objective is to measure the flame temperature and flame position as a function of time until depletion of the deficient reactant (hydrogen) results in extinction of the planar diffusion flame. The fairly hot, soot-free, barely visible nature of a vigorous hydrogen-air flame poses a challenge for diagnostics.

Experimentally, the design of the test chamber is nearly completed. 2-D numerical calculations suggested that about an inch-long baffle extending from the shutter-exit wall perpendicularly into the combustion chamber would help to inhibit corner vortices, formed in the shutter-entrained fluid. Provision for baffles may be incorporated into

the current chamber design. The total "delivery" of fluid entrained by shutter withdrawal is reduced as the withdrawal speed is increased; withdrawal at a constant speed of 250cm/sec is recommended. Heat transfer calculations under typical conditions of the baffle-tip temperature as a function of baffle-thickness, for ascertaining that the baffle-tip temperature does not become too hot to blind the IR cameras, indicate that there is little basis for concern. Detailed drawings of the design, prepared by TRW, are being reviewed by LeRC, and revised until both organizations are satisfied that construction at LeRC may proceed. The chamber is to be created specifically for testing in the NASA 5-second drop tower; this testing is to observe the adequacy of techniques adopted for thin-film removal, subsequent gas ignition, and planar-flame establishment. In particular, TRW and LeRC are designing a rapid-removal-and-storage mechanism for the thin-film separator, involving the use of an inflatable seal. The objective is to permit redeployment of the separator (for another experiment in the 5-second drop tower) without breaking the pressure seal of the container. This would eliminate the need for a new leak-test before every experiment.

The chamber is designed to meet NASA requirements for pressure vessels. For that purpose the results obtained earlier by the Project Scientist, Suleyman Gokoglu, are being utilized. He ran the NASA CEC program extensively for adiabatic flame temperature calculations to clarify safety requirements, as well as to guide the choice of operating conditions. The calculations show that chamber pressure is not expected to exceed 10 atmospheres. The mixture ratios which result in adiabatic flame temperatures between 1800 - 2600_K are identified. The chamber material and wall thickness, and the locations and dimensions of the optical windows for diagnostics, are being selected on the basis of the constraints and requirements for science and engineering. Computer calculations to confirm that the chamber design, including optical-access windows, can withstand (wrt. stress and deflection) the anticipated peak pressure are under way using the ANSYS finite-element structural analysis code. The results so far indicate that the chamber wall and window thicknesses chosen for design are within safe limits.

The conceptual design of experiments to determine the suitable ignition parameters, i.e. minimum and nominal ignition energy, temporal interval for energy deposition and electrode separation distance, are completed. Parts have been ordered for the construction of the experiment. These experiments will also provide assurance for safety that conditions which may lead to detonation are being avoided. A candidate "home-grown" spark-ignition system sent by TRW to LeRC will be used for testing.

For temperature measurement, LeRC completed the detailed design of an experiment to properly calibrate the two candidate techniques selected via the LeRC QFD process: 1) a band-ratio technique using the infrared-emission of the water-vapor product (LeRC's current first choice) and 2) a ceramic fiber emission technique (LeRC's current second choice). LeRC plans to use known-melting-point (pure, single crystal), thin (~100 _m in diameter) and non-emitting, stiff, chemically non-reacting fibers under typical combustion environments planned for _g experiments for the calibration of the band-ratio technique. Parts have been ordered for the construction of the experiment. A Physics Professor from Cleveland State University has been contacted to help the project team in optical engineering and spectroscopical analysis of the experiment.

The current concept for parametric investigation in extended microgravity is for repeated use of a single unit, initially evacuated and sealed, with a thin film in place to divide the contents into two equal subvolumes. Soon before test execution, one control is to initiate and terminate the gradual, simultaneous filling of the half volumes, each half volume being connected to its own 'feed' bottle. This procedure maintains negligible pressure differential across the thin film, yet avoids the problem of hydrogen permeability that would arise if long storage of a gas-filled unit were required. Upon command, chemical "freezing" of the container contents by expansion into a large volume is planned as an option during testing. The outline of the experimental procedure is being updated as an evolving document, as intended. The science requirements are being revisited and refined in conjunction with decisions and clarifications from chamber design, sub-system functional capabilities, experimental procedure and numerical work.

TRW favors composing the chamber for spaceflight of stainless steel, and forming it of two top-hat-configured parts, with a retractable/restorable foil fixed between the two halves by an inflatable seal. TRW favors the use of sapphire needle valves in backfilling the test chamber, to meet the requirement of maintaining "equal" pressure on each side of the thin-film separator as the gaseous compositions are introduced. The maximum allowable pressure difference between the two half volumes after the fill but before the separator is removed is specified. TRW strongly favors early construction and trials of the gas filling hardware to detect any shortcomings in the flow logic, and to gain facility in its operation. Another concern, arising in connection with the repeated use of a single

chamber for parametric testing, is the accumulation of the heat from combustion, in the absence of convective cooling in microgravity. However, the heat from any one test is modest, and is distributed over an apparatus with large thermal inertia. The temporal interval to be allowed for cooling between tests, and the pressure to which the chamber is to be evacuated prior to refilling for the next test in a sequence, are specified. TRW recommends conducting tests with the apparatus in earth gravity, especially with initially highly-stably-stratified contents (hydrogen/helium above oxygen/argon), to demonstrate the rapid onset of Rayleigh-Taylor instability, within about 0.2 seconds or so; such testing affords a very brief interval for observation of a planar diffusion flame, and demonstrates the requirement of prolonged microgravity for sustaining planarity in a virtually strain-rate-free diffusion flame.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/94 EXPIRATION: 7/98

PROJECT IDENTIFICATION: 963-15-00

NASA CONTRACT NO.: NAS3-272

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Fendell, F.E. and Mitchell, J.A., Feasibility of planar, unidirectional-flow diffusion flames in earth gravity. Comb. Sci. & Tech., (October, 1995).

Fendell, F.E. and Wu, F., Unsteady planar diffusion flames: ignition, travel, burnout. Comb. Sci. & Tech., vol. 107, pp. 93-126 (October, 1995).

Fendell, F.E. and Wu, F., Diffusion-flame burning of fuel-vapor pockets in oxidizer for general Lewis numbers. Combustion and Flame, vol. 105, pp. 1-14 (1996).

Fundamental Study of Smoldering Combustion in Microgravity

PRINCIPAL INVESTIGATOR: Prof. A. C. Fernandez-Pello

University of California, Berkeley

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The overall project objective is to increase the fundamental understanding and the prediction of smoldering combustion under normal and microgravity conditions. This in turn will help the prevention and control of smolder originated fires both, in normal gravity and in space-based environments. The specific objectives are to determine the smolder characteristics of a polymeric porous combustible material (polyurethane foam), in a quiescent or convective oxidizing environment, both at normal and micro-gravity.

Task Description:

The project objectives are accomplished by conducting experiments on ground-based and space-based facilities, and by developing theoretical models of the process. The experiments are conducted with polyurethane foam as fuel with mixtures of oxygen/nitrogen as oxidizer. Temperature at several locations of the sample are measured with thermocouples; and the resulting temperature histories are used to obtain the smolder propagation velocity and smolder reaction temperature, as a function of the oxidizer flow velocity and oxygen concentration. The experimental results are used to verify and improve the theoretical models of smolder combustion. Experiments are also conducted to observe the potential transition from smoldering to gas flaming, and to determine the conditions and mechanisms leading to this transition.

Task Significance:

Smolder is important as both a fundamental combustion problem, i.e., the propagation of a heterogeneous, non-flaming, surface combustion reaction through a porous combustible material, and as a fire safety problem, i.e., the production of toxic compounds and the potential initiation of a fire through the transition to flaming. There is a need for further understanding of the problem for better prediction and control of smolder in both normal gravity and microgravity. Furthermore, microgravity introduces additional questions about the transport of mass to and from the reaction, and the transfer of heat from the reaction, that must be resolved in order to predict smolder behavior in a space-based environment.

Progress During FY 1996:

Progress:

Task 1: Ignition Study of Opposed Smoldering (D. Walther)

STS-69 Shuttle GAS Can flight data was received 10/5 from LeRC. The NASA provided data processing/extraction techniques work very well. Plots of sample temperature profiles were constructed and compared to the Flight Simulation Data from NASA Lewis 3/13/95.

Estimates of CO and CO₂ production from the smolder were submitted to NASA Lewis in order to predict span for post combustion gas analysis.

Completion of experiments for paper titled: "An experimental study of smolder ignition". Paper is to be submitted to the Western States Section Combustion Institute Symposium 10/30-1. Paper is co-authored by Ralph A. Anthenien.

Experimental studies have been conducted to determine the initial effects of 40% oxygen concentration upon opposed flow smolder. Preliminary results show that indeed smolder waves can be ignited under rather low flow velocities (forced) 0.05 mm/s.

Several tests were conducted with a pure Nitrogen flush in order to examine the behavior of melting of the polyurethane foam under high heat flux conditions.

A paper entitled "Small Scale Smoldering Combustion Experiments in Microgravity" co-authored by D. Stocker, S. Olson, D. Urban (NASA Lewis Research Center), J. Torero (U. Maryland), and AC. Fernandez-Pello (UC Berkeley) was submitted for review to the 26th International Symposium on Combustion. The paper comments on experiments conducted aboard USML-1 (STS-50) and ground based simulations.

Arrangements were made to analyze the STS-69 gas canisters using Performance Analytical. The bulk gases (CO, CO₂, N₂, and O₂) will be measured using a thermal conductivity analysis. Light hydrocarbons with a GC/FID method. Higher hydrocarbons (C₃ +) will be analyzed using a GC/MS method.

Tests were conducted and analyzed for the possibility of flaming at large oxygen concentrations (40% O₂) and to determine the optimum igniter time for STS-77. It was determined that for the quiescent test case, 1200 seconds of igniter on-time will be optimum.

The opposed flow combustion chamber was rebuilt and cleaned for better reproducibility of results. A control box was built in order to accurately control up to four flow controllers. This box will be used in the variable oxygen concentration cases. Tests are being conducted in order to better understand the ignition characteristics under variable oxygen concentration. Flow rates are 0.1 mm/s during the igniter on-time and 0.7 mm/s during the burn. These flow rates were chosen to compare with previous data.

A revised copy of "Small Scale Smoldering Combustion Experiments in Microgravity", Stocker D.P. et. al. has been submitted to the 26th International Symposium on Combustion, Naples, Italy. A work in Progress Poster has also been submitted to this conference entitled "Smoldering Combustion Experiments in Microgravity". This poster outlines the events of the STS-69 shuttle mission and presents some preliminary findings.

Ignition tests are being conducted under varying oxygen concentrations to determine the effect of O₂ concentration on smolder ignition. Test conditions are 0.1 mm/sec (ignition) / 0.7 mm/sec (burn) velocity, in a downward configuration.

Ignition criteria are being developed for various oxygen concentrations in a opposed flow downward burning configuration. Present tests are being conducted using 40% O₂ at flow velocities of 0.1 mm/sec ignition / 0.7 mm/s burn.

Char samples have been sent to NASA Lewis to be used as post igniter insulation for the STS-77 post flight test simulations.

The work-in-progress poster on smoldering experiments in microgravity has been accepted for presentation at the Symposium.

Results from STS-77 are being cataloged and are, to date:

Chamber A

- smolder velocity: 0.157 mm/s
- smolder temperature: 405-410 C
- sample mass(initial):
- sample mass(after): 37.5 g
- char mass: 14.7 g
- mass lost:

Mission simulation and preliminary testing data has also been examined and cataloged.

Preliminary results of ignition tests conducted at 40% oxygen concentration show a significant decrease in overall ignition time and a reduction in minimum igniter temperature (385 C -> according to expectations. The mass losses show no significant differences. Under no cases did the smolder front die out upon reaching the sample end. All samples were extinguished with nitrogen to quench the forward smolder.

Testing of 30% oxygen concentration is underway at the previous flow conditions (0.1 mm/s ignition / 0.7 mm/s burn).

Ignition tests conducted at 30% O₂ compare favorably with those conducted at both 40% and in air. The parameters that are being controlled are still igniter power and ignition time. Resulting smolder velocities are 0.05 mm/s for the flow parameters of 0.1 mm/sec ignition and 0.7mm/sec burn.

Testing has been conducted under very low flow conditions to determine the limits of ignition due to oxidizer transport constraints. Oxygen concentrations and flow rates were varied from ambient to 100% O₂ and flow velocities ranged from 0.05 mm/sec to 0.125 mm/s. No change in flow velocity was enabled.

Igniter conditions were 75W @ 1250 sec. From these tests, under the lowest velocity (0.05mm/s) ignition did not occur even for 100% O₂. Ignition may be possible in a heat assisted mode for extremely long igniter times. The behavior of the smolder ignition resembles ignition characteristics near the rich flammability limit. Smolder velocities for these cases were approximately 0.035mm/sec near the ignition threshold and showed a slight increase with O₂ concentration.

The poster #201 entitled "Smoldering Combustion Experiments in Microgravity" was submitted to the 26th International Symposium. on Combustion.

The paper entitled "A Novel Application of Ultrasonic Imaging to Study Smoldering Combustion," has been submitted to the 1997 Asia Pacific Conference on Combustion (ASPACC97). This paper outlined the technique used in obtaining the ultrasound images as well preliminary results in obtaining information about the location of the smolder front. This paper was authored by S.D. Tse, R.A. Anthenien, K. Miyaska and A.C. Fernandez-Pello.

Task 2: Forward Smoldering (R. Anthenien)

A paper has been submitted and presented to the Combustion Institute's Western States Section Fall Symposium. This paper reports our findings on the requirements for ignition of a smoldering reaction. A simple model for these requirements was also reported.

Work has begun in conjunction with S. Tse (Task 3) to develop a full three-dimensional tomography system for imaging smoldering combustion in real time. We have also begun testing various closed cell foams for their transmittance of the 40 kHz ultrasound signal being used. The closed cell foam will be used for insulating the foam sample and ensuring that the air flow through the sample is properly controlled.

Relays for the ultrasound speakers have been wired and will be used to sequentially pulse an array of speakers. A new speakers/microphone array holder has been made to scan samples with cross-sections larger than 8 in by 8 in. A 486DX33 with on a PCI motherboard with SCSI controller and hard drive has been acquired for high speed data acquisition and storage. Tests with opposed smolder have been run.

The relay setup has been rewired so that high frequency leakage through the electromechanical switches are negligible. File handling, data massaging and reduction, and preliminary filtering modules have been written and included into a global tomography program with the Abel transform module of S. Tse (Task 3).

Many improvements to the ultrasonic imaging hardware have been made in collaboration with Prof. Miyasaka and S. Tse (Task 3). Most of these improvements have been made to strengthen and clean-up the received signal. Improvements were also made to data storage and handling. New adjustable gain pre-amplifiers have been constructed and installed. These use a wider band op-amp and incorporate a noise filter in the circuitry. The power amplifier driving the speakers has also been modified allowing a driving voltage of up to 80V peak-to-peak. This allows for a higher signal-to-noise ratio in the received signal. New connector cables for the microphones were also constructed out of coaxial cable, further reducing noise. A fast scsi-2 drive was installed in the data acquisition computer increasing the data transfer rate, and a zip drive was purchased and installed allowing all the original data to be put in permanent storage. Additional software improvements and modifications have been made.

Final improvements to the ultrasound imaging hardware have been made. A new amplifier with software selectable gains of 1, 2, 5, and 10 has been constructed and placed in-between the multiplexer and data acquisition board, allowing for optimal data resolution throughout a scan. The preamplifiers have been calibrated for a sequentially

pulsed array of speakers and microphones. Post-processing software has been modified for changes in the data acquisition software (S. Tse, Task3). Tomography tests have been run and the results are good. Additional software filters for the deconvolution are needed to clean up the images.

Several improvements to the data filtering for the ultrasound software have been implemented. These include routines such as allowing for data averaging, and modifications to allow for the use of the array of speakers mentioned previously. Also, a new method, whereby the sample is calibrated by comparing the actual ultrasound transmission data to a computed ideal distribution, is currently undergoing tests for feasibility.

Constructed work in progress poster with S.D. Tse for 26th I.S.C. Entitled "A Novel Technique for Ultrasonic Imaging of Smoldering Combustion." Confirmed that ultrasound attenuation system will work for monitoring progress of combustion front and evolution of resultant char in opposed flow apparatus.

Have performed preliminary examinations of several materials for use in sealing ultrasound speakers from hot gases produced by smolder. The optimum material will be gas tight, perform well structurally at high temperature and have a low attenuation of the ultrasound signal.

The paper entitled "A Novel Application of Ultrasonic Imaging to Study Smoldering Combustion," has been submitted to the 1997 Asia Pacific Conference on Combustion (ASPACC97). This paper outlined the technique used in obtaining the ultrasound images as well preliminary results in obtaining information about the location of the smolder front. This paper was authored by S.D. Tse, R.A. Anthenien, K. Miyasaka and A.C. Fernandez-Pello.

Task 3: 2-D Smoldering with Transition to Flaming (S.D. Tse)

Some preliminary ultrasound scans of foam/char setups have been taken. A picture has been posted on the Microgravity Combustion Lab homepage. A power amplifier has been obtained to drive the speakers so that we can test for better penetration of the insulation material.

Prof. Miyasaka visited for 2 weeks and helped in making considerable improvements to the ultrasound imaging system. We now employ a single set of speaker and receiver scanning through 2 axes, instead of an array of 8 sets scanning only through 1 axis. This modification will increase the spacial resolution of our images, as well as negate interference signals from other speakers previously being driven simultaneously. The speaker can now be driven up to 50V peak to peak using a high gain, low noise, power amplifier obtained from Japan. In addition, pulse signals are sent from the speaker instead of a continuous signal, which remarkably improves the technique by differentiating the actual transmitted signal through the foam/char from reflections and other interference signals. The time constant on the rms converter has been reduced to less than that of the period of a single 40kHz pulse so that we can save the entire waveform (on the order of a millisecond) received by the receiver. With the ultrasound frequency remaining at 40kHz, we need a high speed A/D board which can take data at least 80kHz so that we can reconstruct the received waveform. The board has been ordered and should arrive in a week. In addition, the received waveform is superimposed along with the original pulse train from the speaker so that we can measure the time delay between a sent and received signal, giving us some indication of the temperature in the foam/char via the variation of sound speed with temperature. New experimental containers have been built for the foam/char, consisting now of a wire mesh (for rigidity) and fiberfrax paper (for insulation and species impermeability). These materials allow for better ultrasound penetration and detection. Furthermore, a square, ceramic honeycomb igniter replaces the original circular one. The combustion wind tunnel has been slightly modified to account for all of these changes.

The high speed A/D board arrived and has been employed to take data at 4 microseconds intervals. Presently, we save an entire waveform for each ultrasound scanned location. Software has been written which controls the microphone/speaker scanning and data acquisition. Experiments have been run using the new ultrasound imaging apparatus. Data still needs to be analyzed; however, cursory inspection of the real time ultrasound waveforms suggests that the char continues to react and become more permeable after the smolder front has passed.

Additional experiments have been run with local gas probing, with subsequent gas analysis by gas chromatography. These results, in conjunction with data from ultrasound imaging, have been submitted for presentation and publication at the 26th International Symposium on Combustion to be held in Naples, Italy, summer 1996.

Work has begun on perfecting the ultrasound tomography system. An array of speakers/microphones will be used to reduce scanning time. All waveforms will be saved and post-processed using tomography filters. Tests have been run to determine optimum sample size without any insulation for smoldering tomography. It has been found that downward natural opposed smoldering gives a distinct smolder front that can be well tracked by the present ultrasound imaging setup. The goal is to have a 3-D tomography of a symmetrical smoldering sample in time. The sample will be cylindrically shaped without any protective insulation. The results of permeability and temperature field evolution will be sent to a technical journal for publication.

A program module with the Abel transform (for doing 3-D tomography of symmetrical sample) has been written. Scans of a sample with a prescribed smolder front have been made. Preamplifier gains from the microphone were increased for transmission signals.

Prof. Miyasaka from Fukui University visited from April 3 to April 19, and many improvements to the ultrasound hardware have been made. A new function generator with a programmable crystal oscillator has been acquired and gives a very stable 40kHz signal. The old function generator now triggers wavetrain-pulses at 50Hz (20ms between pulses allows for better dissipation of reflected and interference signals before the next pulse; in addition, the speakers can be driven with more power during a wavetrain-pulse without overheating). An amplifier has been added between the multiplexer and data acquisition board for better gain adjustment of the received waveform. The data acquisition board is now triggered by the 50Hz square-wave signal from the old function generator, resulting in reduced data storage and easier software identification of peaks in received signals. All work was done in collaboration with R. Anthenien (Task 2) and additional improvements to the system are documented in that section. Preliminary tomography tests have been run. Additional software improvements and modifications have been made.

The symposium paper, "Controlling Mechanisms in the Transition from Smoldering to Flaming of Flexible Polyurethane Foam," has been accepted for publication and oral presentation. The manuscript has been revised for reviewer's comments and resubmitted. A work-in-progress poster entitled, "A Novel Technique for Ultrasonic Imaging of Smoldering Combustion," with R. Anthenien, K. Miyasaka, and A.C. Fernandez-Pello has been submitted to the symposium.

More improvements to the ultrasound imaging hardware have been made in collaboration with R. Anthenien (see task2). This should be the last of the hardware modifications. The ultrasound data acquisition software has been modified to control an array of sequentially pulsed speakers and microphones. In addition, a gain selecting algorithm for amplification of the received signal has been incorporated. Duplicate tests of the experiments presented in the symposium paper have been made. The images are now much better, considering all of the hardware and software improvements. In fact, these tests indicate that it is now possible to track the progress of a forward propagating smolder wave, which was previously difficult due to the blurring of the smolder zone.

The work-in-progress poster on the ultrasonic imaging technique has been accepted for presentation at the Symposium.

S. Tse presented the paper, "Controlling Mechanisms in the Transition from Smolder to Flaming of Flexible Polyurethane Foam," and the work-in-progress poster, "A Novel Ultrasonic Imaging Technique for Smoldering Combustion," at the 26th International Symposium on Combustion, in Naples, Italy.

Reply to comments from the Symposium presentation have been submitted.

A paper documenting the ultrasound technique has been submitted to ASPACC97.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	1
PhD Students:	3	PhD Degrees:	1

TASK INITIATION: 3/94 **EXPIRATION:** 3/97**PROJECT IDENTIFICATION:** 963-22-05-05**NASA CONTRACT NO.:** NAG3-125**RESPONSIBLE CENTER:** LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Shultz, D.A., Matkowsky, B.J., Volpert V.A., and Fernandez-Pello, A.C., Forced forward smolder combustion. Combustion and Flame, (1996).

Torero, J.L., and Fernandez-Pello, A.C., Forward smolder of polyurethane foam in a forced air flow. Combustion and Flame, (1996).

Presentations

Anthenien, R.A., Walther, D.C., and Fernandez-Pello, A.C., "An experimental study of smolder ignition of polyurethane foam." Western States Section/The Combustion Institute, 1995 Fall Meeting, Stanford University, Stanford, CA, October 31, 1995.

Stocker, D.P., Olson, S.L., Urban, D., Torero, J.L., Walther, D., and Fernandez-Pello, A.C. "Small scale smoldering combustion experiments in microgravity." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28-August 2, 1996.

Tse, S., Anthenien, R., Miyasaka K., and Fernandez-Pello, A.C., "A novel technique for ultrasonic imaging of smoldering combustion." 26th International Symposium on Combustion, August 2, 1996.

Tse, S.D., Fernandez-Pello, A.C., and Miyasaka, K., "Controlling mechanisms in the transition from smoldering to flaming of flexible polyurethane foam." 26th International Symposium on Combustion, (in press 1996).

Walter, D., Urban, D., and Fernandez-Pello, A.C., "Smoldering combustion experiments in microgravity." 26th International Symposium on Combustion, August 2, 1996.

Flammability Diagrams of Combustible Materials in Microgravity

PRINCIPAL INVESTIGATOR: Prof. A. C. Fernandez-Pello

University of California, Berkeley

CO-INVESTIGATORS:

Quintiere, J.G.
Torero, J.L.

University of Maryland
University of Maryland

Task Objective:

The proposed research program will study the effects of microgravity on the flammability diagrams of solid combustible materials, and the fire properties derived from them. The final objective of the research is to develop a new flammability apparatus that would better reflect the potential ambient conditions of space-based environments, i.e., microgravity, low velocity flow, oxygen concentrations slightly below and above that of air, and use it to obtain more appropriate flammability diagrams for practical materials (plastics, cable jackets, electronic board, etc.) that will be found in space-based facilities.

Task Description:

The LIFT, "Lateral Ignition and Flame Spread Test", ASTM E-1321, apparatus, although not considered a general fire test method, can provide key information about the ignition and flame spread characteristics of a material, including critical radiant flux for ignition, ignition delay, ignition temperature, flame spread rate constants, and extinction limit, the most important characteristics with regard to the initiation of a fire in a space facility. These fire properties are extracted from the "Flammability Diagram" of the material, that are constructed from the data obtained from the LIFT test. The LIFT apparatus, however, relies on gravity for the transport of heat and mass, and consequently cannot be used in microgravity.

A new test apparatus, FIFST, for "Forced Flow Ignition and Flame Spread Test", will be designed for microgravity. It will be based on forced flow transport of heat mass, and will provide information about the ignition time and flame spread properties of the material as a function of an externally applied radiant flux. The apparatus will be used to measure in microgravity, the ignition delay and flame spread rate (opposed and concurrent) of combustible materials as a function of the external radiant flux, and for varied oxidizer flow velocity and oxygen concentration. Since the theoretical background of ignition and flame spread is basically the same for forced and natural convection, the LIFT and FIFST flammability diagrams should be similar, although some of the fire properties obtained with the latter will be dependent on the velocity and oxygen concentration of the flow. Comparison of the flammability diagrams of a few well characterized materials, obtained in the LIFT and FIFST apparatus in normal gravity, and in the FIFST apparatus in microgravity, will provide information about the effects of gravity on the fire properties of materials as given by these diagrams. The results of these studies will be used to develop a conceptual design for a test of the flammability of materials in microgravity. It is envisioned that it could result in a standard testing procedure to determine the fire hazard characteristics of materials in spaced based environments.

Task Significance:

The strong possibility of an accidental fire occurring in a space-based facility during a long mission, is a primary safety concern, and consequently it is of critical importance to characterize the fire properties of materials that are, or will be, used in these facilities. Currently there is no testing methodology that specifically addresses the fire properties of materials in ambient conditions expected in a space-based facility. NASA is using tests, such as the NASA Upward Flame Propagation test, that are based on the common belief that a material in reduced gravity burns less than in normal gravity. Although this is probably true in a quiescent environment (where diffusion is the only transport mechanism), space environments generally have low velocity air currents that are produced by their heating and ventilation systems (of the order of 0.1 m/sec), and recent experiments of flame spread in microgravity show that at these low velocities, the ignition is vigorous, the flame spread is higher, and the limiting oxygen concentrations for spread are lower than in normal gravity. Furthermore, the CO removal and oxygen replenishing system in such a facility, would cause fluctuations in the ambient oxygen concentration above and below that of air, which would also affect the burning of the materials. Therefore it is critical to establish a test for fire conditions that will properly represent the fire hazards that are expected to be encountered in a space facility.

Progress During FY 1996:

The proposed program is being distributed between the two proposing institutions into the following main tasks: normal gravity related activities with the FIFST apparatus will be done at U.C. Berkeley, and with the LIFT at the University of Maryland. Microgravity related activities will be done at the University of Maryland. The know-how gained by the Principal Investigator in the design and utilization of similar microgravity apparatuses is being used in the design and construction of the FIFST apparatus to be used in microgravity tests. A kickoff meeting with NASA team personnel and the PI and Co-I was held, resulting in the outline of specific operational and measurement requirements for the space-based experiments. The research program is now planned in progressive stages that are determined by the characteristic times of the specific fire conditions under study (ignition delay or flame spread rate), and the microgravity time provided by the different experimental facilities available at NASA. The tests that will cover those sections of the flammability diagram that require short periods of microgravity will be conducted at the NASA Lewis Drop Tower, and in the DC-9 parabolic flight. The completion of the diagrams will require tests in facilities with longer periods of microgravity, such as sounding rockets, the Space Shuttle or the Space Station. These experiments will be done in successive extensions of the program, if approved. The analysis and comparison of the data will be carried out by the close interaction of the investigators from both institutions.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 2
PhD Students: 1

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 993-15

NASA CONTRACT NO.: NCC3-478

RESPONSIBLE CENTER: LeRC

Ignition and the Subsequent Transition to Flame Spread in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Takashi Kashiwagi

National Institute of Standards and Technology

CO-INVESTIGATORS:

Baum, H.

National Institute of Standards and Technology (NIST)

MacGrattan, K.

National Institute of Standards and Technology (NIST)

Task Objective:

The objective is to conduct experiments of radiative ignition followed by transition to flame spread over various, different combustible solid surfaces in microgravity in order to understand the transition mechanisms from the ignition to subsequent flame spread, and to determine the effects of preheating, oxygen concentration, external flow velocity, geometrical configuration, and sample materials on the transition and flame spread characteristics.

In addition, theoretical models which describe ignition and subsequent transition to flame spread in two and three-dimensional configurations as well as an axisymmetric narrow tube configuration in a microgravity environment will be developed and compared with experimental results to determine the accuracy of the calculated results and to examine the chemical and physical processes used in the models.

Task Description:

This study consists of a theoretical part and an experimental part. The latter has two different flights; one is a Glovebox experiment called RITSI (flew on USMP-3, STS-75 in Feb. 1996) and the other is a future flight experiment being called TIGER-3D which is currently in the definition stage. A numerical model which can calculate time-dependent phenomena of ignition and subsequent flame spread over a thin cellulosic paper has been developed in three different configurations -- axisymmetric, two and three-dimensional Cartesian. Ignition can be initiated locally by an external thermal radiation or a heated wire.

The unique feature of this study is that localized ignition is initiated in the middle part of the sample instead of at the end of a sample. Therefore, there could be two possible flame fronts; one travels toward upstream and the other toward downstream under an external wind. A slow external wind up to 5 cm/s is studied in the calculation. It is planned that this model will be extended to apply to a thermally thick material, a plastic material, and smoldering. The results can be directly compared with the experimental results which will be obtained in the RITSI and TIGER-3D flight experiments.

Task Significance:

For the first time, it is possible to study the transition from a radiative ignition to flame spread in the absence of overwhelming buoyant convection. The elimination of natural convective flow in the microgravity experiment simplifies both the formulation and subsequent computation of these time-dependent, three-dimensional problems that include other complexities such as finite rate chemical kinetics in both the gas and solid.

Progress During FY 1996:

A paper was written to determine the effects of external flow on ignition and subsequent flame spread in microgravity. The three experiments with external velocity of 0 cm/s, 2 cm/s, and 5 cm/s in 50% oxygen atmosphere in the JAMIC I tests were used for the experimental analysis and three-dimensional calculations were conducted for the three velocities. Both experimental data and the theoretical predictions show that there is little effect of the flow velocity on ignition delay time but it has significant effects on upward flame spread rate (in opposed mode) and also on downstream flame front behavior (in concurrent mode). The paper was submitted to the Twenty-Sixth International Combustion Symposium and it was accepted for presentation and publication in the proceeding.

As described below, radiative ignition of filter paper by a lamp appears to be easier in microgravity than in normal gravity (horizontal beam normal to a vertical sample). This could be due to buoyancy induced flow of hot degradation products moving away from the irradiated area in normal gravity. On the other hand, in microgravity the hot degradation products stay near the irradiated area and mix with air to cause spontaneous ignition. In order to

prove this theory, our two-dimensional numerical code is being modified to include gravity. The effects of the diameter of the external radiant beam on ignition in normal gravity and their comparison in microgravity will be determined.

RITSI: A total of 25 experiments were completed in the glovebox of Columbia (STS-75) in the USMP-3 flight; 15 of them were required samples and the remainder were extra samples. The first surprise was that radiative ignition by the lamp followed by successful transition to flame spread occurred in all experiments except at zero external velocity. We have never observed the transition to flame spread in air at normal gravity using ignition by the lamp only. This indicates that the transition tends to be easier in microgravity than in normal gravity.

Another interesting observation is that the flame does not spread downstream at all in air (along the direction of the external flow) following ignition at the middle part of a sample. However, the flame spreads upstream with a fan shape (fastest in the direction parallel to the incoming flow and gradually slowing down to zero in the direction normal to the incoming flow). With an increase in the incoming flow velocity, the spread angle increases due to an increase in oxygen supply rate. These two trends are completely opposite to those observed in normal gravity (spread is much more rapid downstream and the spread angle narrows with an increase in the incoming flow velocity). The lamp ignited the sample more consistently than the heated wire which depends on its contact to the sample and also its expansion during heating makes ignition not always uniform. We used the lamp as an ignition source for all the extra samples. Three narrow samples (4 cm wide instead of the regular 10 cm wide sample) with two open sides were used to examine flame spread characteristics along the open edges. The results show that once the flame reaches the edge it spreads much faster than it does along the center of the sample. With 2 cm/s external flow, the flame only spreads upstream along the edges but above 3.5 cm/s flow the flame spreads both upstream and downstream along the sample edges. Downstream edge flame spread rate might be the highest. We studied the effects of a corner on flame spread for tests #23 and #25 using a 90 degree bend at one side of the sample. Slowdown of approaching flame toward the corner was observed but flame coming from the open corner side (270 degree) appeared and it spread rapidly along the open corner. These results show that there are significant effects of the three-dimensional geometrical configuration on flame spread, which can not be observed by a two-dimensional configuration. Since flame spreads much faster than it does in the two-dimensional configuration, these three-dimensional flame spread configurations would be more relevant to fire safety in microgravity.

Four smoldering experiments were conducted with ignition initiated by the lamp. Although a ring shaped smoldering front was observed in normal gravity, an unexpected, very complex char pattern with smoldering fronts forming diverging branches was observed. Higher external flow velocity tends to increase the number of branches and also increases the number of bifurcations from each branches. It is not clear what causes this complex shape. One possible explanation is that there is some non-uniformity in thickness in the filter paper. Since potassium ions were heavily doped into the samples (more than needed to make sure that smoldering rate does not depend on the ion concentration), we tend to believe that this phenomena would not be caused by a non-uniformity in ion concentration in the sample. Since smoldering induces roughly 20 cm/s buoyancy induced flow in normal gravity, it appears that some non-uniformity of the sample tends to be suppressed in normal gravity. However, in microgravity it appears that the flow velocity up to 5 cm/s does not suppress it. We are not sure what causes the observed smoldering spread pattern and further study is needed to examine the uniformity in the sample and more experiments in microgravity are needed to clearly understand the observed phenomena. Overall, the experiments were a great success and we have a lot of new data and some of them are quite surprising and puzzling.

JAMIC II: Shortly after the RITSI experiment, Sandra Olson and Carl Fritz went to JAMIC and conducted a total of 20 experiments with Professor Osamu Fujita and his graduate student, Masao Kikuchi. The external flow velocity was extended to 10 cm/s and five tests were conducted with a new sample of thin polyethylene sheet. An IR camera was used to determine the feasibility of the surface temperature distribution. A majority of the experiments were conducted in 35% oxygen atmosphere with five experiments in 50% oxygen and two experiments in air. Although detailed analysis of the experimental results is in progress, flame spread over a thin PE sheet appears to be mainly controlled by rolling up of the melting PE layer which appears to drag a blue flame front. Thus, it appears that the effects of the external flow does not appear to be as important as for the filter paper.

TIGER-3D: DC-9 flight tests were conducted in June and July. Data analysis is underway, and additional tests are planned for September. A Science Concept Review (SCR) will be held in October.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 11/94 EXPIRATION: 11/98
PROJECT IDENTIFICATION: 963-15-OB
NASA CONTRACT No.: C-32001-R
RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

McGrattan, K.B., Kashiwagi, T., Baum, H.R., and Olson, S.L., Effects of ignition and wind on the transition of flame spread in a microgravity environment. Combustion and Flame, (October, 1995).

Presentations

Kashiwagi, T., McGrattan, K.B., Olson, S.L., Fujita, O., Kikuchi, M., and Ito, K. "Effects of slow wind on localized radiative ignition and transition to flame spread in microgravity." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28-August 2, 1996.

The High-Lewis Number Diffusive-Thermal Instability in Premixed Gas Combustion and Low Temperature Hydrocarbon Oxidation and Cool Flames

PRINCIPAL INVESTIGATOR: Dr. Howard G. Pearlman

University of Southern California

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This effort encompasses two distinct investigations with complimentary but different objectives. The first effort will be directed at developing a greater understanding of the High-Lewis number diffusive-thermal instability. The effects of Lewis number, gas mixtures, heat loss and the role of additives/inhibitors will be studied in both normal and reduced gravity. The system in which this instability will be investigated is a large diameter tube filled with a mixture of known gases which are ignited on one end. The instability manifests itself as the flame propagates from one end of the tube to the other. For the effect of gravity to be small, the diameter of the tube must be less than that for which the flame tends to extinguish due to conductive heat loss. In most practical scenarios, that condition is not met and reduced gravity testing must be conducted.

The second effort is aimed at understanding low-temperature oxidation reactions and cool flames. This investigation will be conducted in both open and closed vessels into which a mixture of known gases is introduced. The chamber and thus the gases are then heated until a reaction, typically not classified as ignition, is initiated. In these systems, buoyancy alters the hydrodynamic, thermal and concentration fields. In turn, this changes the flame shape and reaction rate. Hence, the requirement for reduced gravity. Since the time required for reaction initiation can be on the order of minutes, these experiments must be performed on orbit. Therefore, the current objective for the PI on this portion of the project is to provide technical direction to the engineering teams designing and fabricating the breadboards of critical systems prior to the Science Concept Review (SCR). At SCR, results from these tests will help determine whether or not the project is manifested for flight.

Task Description:

In order to understand the effect of Lewis number on the diffusive-thermal instability, several parameters will be independently varied. First, the Lewis number, which is the ratio of the thermal to mass diffusivity, will be varied by either changing the diluent or using fuels with increasing molecular weight and hence lower mass diffusivities. However, mixture ratios may affect flame propagation and stability independent of Lewis number effects. Therefore, an effort will be made to hold the Lewis number constant while varying the fuel concentration. Heat loss can also affect the propagation and stability characteristics of a flame. To study this parameter, the Lewis number will be held constant and propagation tubes of differing diameter used. In small diameter tubes, conductive loss is the dominant mechanism whereas flames in larger tubes are mostly affected by radiative loss. As part of the latter investigation, the fuel will be seeded with inert particles to absorb radiation ahead of the flame and extend the limiting concentration of the scarce component at the lean flammability limit to lower values. Since a uniform concentration of particles is required for a meaningful interpretation of the results, reduced gravity will be utilized to insure that the seed does not settle out of the gas.

Additional effects to be studied include pressure, which can change the thermal diffusivity of the mixture and additives which can remove radicals from the combustion reaction and thus change the thermal feedback.

The flight definition project will require the construction and evaluation of subsystems that have been identified by NASA LeRC personnel as requiring proof-of-concept prior to SCR. The majority of this effort will be conducted by NASA engineers with consultation from the PI via the LeRC Project Scientist.

Task Significance:

Instabilities similar to the diffusive-thermal instability to be studied under the first part of this investigation have been observed in combustion synthesis of materials. In such cases, burning of a solid is involved, which mandates that the combustion can only be understood on the surface of the material. Since the current investigation involves gaseous components, transport throughout the system can be observed and parameters more easily varied. The

knowledge thus gained, which is not available in any other configuration, should be directly applicable to combustion synthesis of materials.

The cool flame investigation is aimed at understanding processes that occur leading to spontaneous ignition. As such, the investigation will lead to an increased understanding of the physics behind knock in engines. Such an understanding is lacking in current combustion theory and fuel manufacturers have avoided the problem by using additives.

Progress During FY 1996:

Following the announcement of funding, a team was organized at NASA LeRC to develop engineering requirements prior to the design and fabrication of the critical breadboards required to demonstrate feasibility. The PI met with the team on an *ad hoc* basis to provide his assessment of the results. The team completed its work and submitted a report describing the science and technology demonstrations required for a successful SCR. A breadboard engineering team is currently being assembled.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/96 EXPIRATION: 9/00

PROJECT IDENTIFICATION:

NASA CONTRACT No.: NCC3-501

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Pearlman, H. Excitability in high-Lewis number premixed gas combustion. Combustion and Flame Paper No. 1612, (accepted April, 1996).

Pearlman, H., Stocker, D., Gotti, D., Urban, D., Ross, H., and Sours, T. Demonstrating reduced gravity. The Physics Teacher, vol. 34, No. 3, 172-176 (1996).

Presentations

Pearlman, H. "An excitable premixed gas reaction." Department of Chemistry, West Virginia University, Morgantown, WV, August 8, 1996.

Studies of Premixed Laminar and Turbulent Flames at Microgravity

PRINCIPAL INVESTIGATOR: Prof. Paul D. Ronney

University of Southern California

CO-INVESTIGATORS:

Wu, M.-S.

University of Southern California

Task Objective:

The objective of this work is to study the effects of gravity-induced buoyancy on the combustion limits of premixed gas flames. The following sub-tasks have been pursued during FY96:

- (1) Low-Lewis number flame structure and stability at microgravity.
- (2) Study of the high-Lewis number diffusive-thermal instability in premixed gas combustion.
- (3) Experimental simulation of combustion processes using autocatalytic chemical reactions.

Task Description:

For task 1, we are studying flames in a variety of gas mixtures having low Lewis number (Le) in drop tower and aircraft tests, particularly those exhibiting stationary spherical flame structures (flame balls). These tests are in support of the Structure Of Flame Balls At Low Lewis-number (SOFBALL) flight experiment to be performed using the Combustion Module-1 (CM-1) hardware on Space Shuttle Mission MSL-1 in March 1997. Numerical modeling of flame balls is being performed to refine the flight test matrix and provide a theoretical comparison to the experimental results.

For task 2, we are studying flames in gas mixtures having high Lewis number (Le) in laboratory and drop tower tests. These experiments form a companion experiment to those in task 1.

For task 3, we have introduced the use of aqueous autocatalytic chemical fronts for simulating premixed gas flame fronts. The aqueous fronts propagate at steady rates but are unaffected by heat losses, have practically no change in transport properties across the front and exhibit very small thermal expansion. Three flows have been employed: Taylor-Couette and Capillary-Wave flows to produce nearly isotropic turbulence, and Hele-Shaw flow to study buoyancy-driven front propagation in a flow described by linear equations.

Task Significance:

It is anticipated that the results of these studies will lead to an improved understanding of the fire hazards that may exist in orbiting spacecraft and of ways to minimize these hazards. Furthermore, such studies may lead to an improved understanding of the mechanism of combustion limits in Earth-based devices, which in turn could lead to the development of cleaner and more efficient engines through the use of lean premixed combustors.

Progress During FY 1996:

1. Low-Lewis number flame structure and stability at microgravity

Numerical simulation of flame balls were developed for comparison with the SOFBALL flight experiments and for a determination of the range of potential physically observable flame balls. The results indicate that the chemical models employed affect flame ball properties substantially. Thus, results of flame ball experiments may provide a new basis for testing these models at low flame temperatures. In addition, the far-field radiative loss is found to affect the behavior of flame balls in a manner very different from propagating planar flames. Only with far-field losses are oscillatory solutions and a dynamic extinction limit predicted in addition to the static limit. Also, the model predicts a decreasing flame ball radius for decreasing Lewis number and mole percent of fuel, as is seen experimentally.

An important part of flame ball modeling is the accurate prediction of the flame ball emission intensity profile. The intensified CCD cameras used in the experiment detect radiation from 400 to 900 nm. For comparison of the

experimental data with numerical simulation results, emissivities of the gases in the visible region, which are several orders of magnitude weaker than in the infrared and are usually neglected, are needed. We are in the process of developing a model for the calculation of the emissivity of gases in the 400 to 900 nm region that considers a multi-band structure as an assembly of many individual lines. Fundamental data available in the HITRAN data base from the US Air Force are used to calculate the spectral bands and emissivities.

Five weeks of test were performed on NASA's DC-9 research aircraft in support of the SOFBALL flight experiment using a flight-like combustion chamber, ignition system, and instrumentation. The results enabled selection of the gas compositions, spark ignition energies, and diagnostic settings for the space experiment. Analysis of radiometer data using the flame ball position determined from video images was done. Additional analysis of the flame ball position was begun using a Stereo Imaging Velocimetry algorithm developed by NASA Lewis.

2. High-Lewis number premixed gas combustion

During the past year, a tremendous amount of progress has been made towards understanding the high-Lewis number, diffusive-thermal instability in premixed gas combustion. Specifically, experimental evidence of pulsating and traveling wave instabilities was observed in normal gravity flames (burner-stabilized and freely-propagating) in a variety of mixtures including methane, propane, butane, heptane, octane and nonane diluted with oxygen and helium. Additional experiments have also been performed to rule out the possibility that these instabilities are purely chemical, acoustic, or hydrodynamic. All of the results support the contention that the observed instabilities are, in fact, diffusive-thermal in nature, which makes this study the first definitive evidence to support the existence of high-Lewis number diffusive-thermal instabilities in a gas-phase, exothermic reaction.

Moreover, similar dynamical behavior in aqueous, reactive systems (e.g., Belousov-Zhabotinskii reaction) and solid-phase combustion synthesis (SHS) suggests that the observed instabilities at high-Lewis number are perhaps a more general feature of reactive-diffusive systems that include premixed gas-phase combustion. Since thermal feedback, rather than molecular diffusion, can provide the essential feedback to sustain the autocatalysis, the results obtained suggest that excitable dynamics and spontaneous pattern formation can (and do) occur in premixed flames provided they are sufficiently far from equilibrium.

3. Experimental simulation of combustion processes using autocatalytic chemical reactions

Aqueous autocatalytic chemical reactions can be used to study buoyancy effects on propagating fronts using a two dimensional Hele-Shaw apparatus in which the flow is created solely by buoyancy. This system represents the simplest possible realization of the interaction of a propagation front under the influence of buoyancy. Digital video images were acquired of the propagation. A program was developed to measure the curvature of the propagation front. The results showed the propagation to be a function of the product of Grashof, Schmidt, and the inverse of Peclet numbers, and suggests a rather simple description of the role of buoyancy on the front propagation in this simple chemical and hydrodynamical system. Some instabilities like a fingering phenomenon were observed.

To complement the above task, a joint research program with Prof. Jerry Gollub of Haverford College was initiated for the study of front propagation in a two-dimensional array of vortices generated using a magnetohydrodynamic flow system.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	12	BS Degrees:	10
MS Students:	3	MS Degrees:	2
PhD Students:	3	PhD Degrees:	1

TASK INITIATION:	3/91	EXPIRATION:	12/98
PROJECT IDENTIFICATION:		962-22-05-06	
NASA CONTRACT No.:		NAG3-152	
RESPONSIBLE CENTER:		LeRC	

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Pearlman, H., Excitability in high-lewis number premixed gas combustion. *Combustion and Flame*, (1996).

Shy, S. S., Jang, R. H., and Ronney, P.D., Laboratory simulation of flamelet and distributed models for premixed turbulent combustion using aqueous autocatalytic reactions. *Combustion Science and Technology*, vol. 113-114, 329-340 (1996).

Presentations

Abid, M. and Ronney, P.D., "Buoyancy effects on propagating chemical fronts in aqueous solution." 48th Annual Meeting, Division of Fluid Dynamics, American Physical Society, Irvine, CA, November 19-21, 1995.

Pearlman, H., "Spiral wave and target patterns on the surface of a freely-propagating premixed gas flame." Dynamics Day Workshop, Houston, TX, January 3-6, 1996.

Pearlman, H., "Excitability in high-lewis number premixed gas combustion." West Virginia University Department of Chemistry, August 8, 1996.

Pearlman, H., "Excitability in High-Lewis number premixed gas combustion." West Virginia University Department of Chemistry, August 8, 1996.

Ronney, P.D., "Combustion at zero gravity." 36th Israel Annual Conference on Aerospace Sciences, Haifa, Israel, February 21-22, 1996.

Ronney, P.D., "Dynamics and pattern formation in propagating chemical fronts in buoyant and turbulent flows." 15th Dynamic Days, Houston, Texas, January 3-6, 1996.

Ronney, P.D., "Combustion experiments on spacelab mission MSL-1." 6th International Space Conference of Pacific Basin Societies, Marina del Rey, CA, December 6-8, 1995.

Ronney, P.D., "Dynamics and pattern formation in propagating chemical fronts in buoyant and turbulent flows ." 15th Dynamics Days Texas, Houston, TX, January 3-6, 1996.

Ronney, P.D., "Dynamics and pattern formation in propagating chemical fronts in buoyant and turbulent flows." California Institute of Technology, May 17, 1996.

Ronney, P.D. and Abid, M., "Buoyancy effects on propagating chemical fronts in aqueous solution." 48th Annual Meeting, Division of Fluid Dynamics, American Physical Society, Irvine, CA, November 21-22, 1995.

Ronney, P.D., and Wu, M.-S., "Numerical simulation of flame ball structure and stability." 6th SIAM Conference on Numerical Combustion, New Orleans, LA, March 4-6, 1996.

Ronney, P.D. and Wu, M.-S., "Numerical simulation of flame ball structure and stability ." 6th SIAM Conference on Numerical Combustion, New Orleans, March 4-6, 1996.

Ronney, P.D. and Zhu, J.-Y., "Numerical simulation of buoyant chemical front propagation in Hele-Shaw flow." 6th SIAM Conference on Numerical Combustion, New Orleans, LA, March 4-6, 1996.

Ronney, P.D. and Zhu, J.-Y., "Numerical simulation of buoyant chemical front propagation in Hele-Shaw flow." 6th SIAM Conference on Numerical Combustion, New Orleans, March 4-6, 1996.

Wu, M.S., Ronney, P.D., Colantonio, R.O., VanZandt, D.M., "Detailed numerical simulation of flame ball structure and dynamics." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28-August 2, 1996.

Ignition and Flame Spread of Liquid Fuel Pools

PRINCIPAL INVESTIGATOR: Dr. Howard D. Ross

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

Sirignano, W.A.
Miller, F.J.

University of California, Irvine
Case Western Reserve University

Task Objective:

The Spread Across Liquids (SAL) experiment will characterize how flames spread across liquid pools in a microgravity (μg) environment, compared with tests at Earth's gravity and with a state-of-the-art numerical model developed specifically for this problem.

Task Description:

In 1991, NASA held a peer review to determine whether to proceed to a space-based experiment with this study. A matrix of 10 tests was proposed at that time which spanned a range of opposed air speeds, concurrent air speeds, and fuel types. Mainly because of the relatively large hazard associated with the required amount of fuel for this microgravity combustion science experiment, we proposed using a sounding rocket instead of the Shuttle for the longer duration microgravity experiments. It was decided at that time by NASA Headquarters to proceed with 3 of the 10 tests and defer a decision on the remaining tests for the following reasons: (a) the experiment required an untried and undeveloped technology of completely filling a tray with liquid fuel in microgravity and then maintaining that liquid in the tray during ignition and flame spread; (b) the experiment was proposed for a sounding rocket, which represented an untested platform for microgravity combustion science experiments; and (c) the experiment involved a set of advanced diagnostics which had not yet been attempted in microgravity. In addition, recommendations were made on the direction of development of the predictive, 2-dimensional, transient numerical model and verification should proceed.

The three tests -- all involving opposed air flow for a single pool depth and fuel type -- have now been performed. All were completely successful in returning the desired science data, in demonstrating an ability to manage the liquid fuel, in measuring temperature and velocity fields with advanced, non-intrusive diagnostics, and of demonstrating that sounding rockets provide a comparatively inexpensive means to fly a very complex, and potentially hazardous, experiment and to perform reflights at very low additional cost.

Task Significance:

The modeling and experimental data provide a more complete understanding of flame spread (a relatively immature area of combustion science) and add to our knowledge about on-orbit and Earth-bound fire behavior and fire hazards. SAL was the first sounding rocket-based, microgravity combustion experiment in the world. Since then, both ESA and other NASA projects have selected sounding rockets as platforms for their combustion experiments. Most importantly, the experiments and modelling yielded considerable new understanding of -- and several new questions about -- flame spread across liquids.

Progress During FY 1996:

UNIFORM FLAME SPREAD

One of our goals has been to resolve contradictions in the literature through experiments in $1g$ and in μg as well as to perform related numerical modelling. The results of our measurements in $1g$ can be summarized as: 1) high spatial and temporal resolution is needed to measure the temperature and velocity fields near the surface for uniform flame spread; 2) the pool is not truly quiescent prior to ignition; 3) the use of measurement methods based on refractive index, e.g. Rainbow Schlieren Deflectometry and Holographic Interferometry, to infer the existence or extent of convective flow for this kind of flame spread problem can be misleading; 4) preheating is confined to a very short distance ahead of and below the flame; and 5) the liquid convection is confined to a very thin layer and, since it is overtaken by the flame, cannot be the only preheating mechanism (in flame-fixed coordinates the flow appears to be toward the flame). Thus, a second mechanism such as gas-phase conduction must be playing a role in this scale experiment.

Our numerical model was then used to generate detailed maps of the velocity and temperature fields similar to those obtained from experimental results. In general agreement with Ito et al. (1991) and more closely with our experiments, the model predicts the existence of liquid-phase flow slightly ahead of the uniformly spreading flame. In contrast to our experiments, however, the predicted liquid surface velocity near the flame leading edge is always greater than the flame spread rate. The flame spread rate and the region ahead of the flame where liquid flow is discernible are well predicted by the model.

PULSATING FLAME SPREAD BEHAVIOR

Of special interest to this work is the determination of whether, and under what conditions, pulsating flame spread can and will occur in microgravity in the absence of buoyant flows in both phases. One question, which remains an issue in these investigations, is whether pulsations may be induced in μg by the presence of a forced opposed air flow. As described below, the model predicts this kind of behavior, however the experiments have not yet confirmed it. Hypotheses on the differences between experiments and modelling will be discussed later; the proposed sounding rocket reflight experiments will be able to test these hypotheses.

An additional question relates to the direction of forced air flow. When there is sufficient flow in the direction concurrent with the flame spread, there is no recirculation cell in the gas phase. If the model is correct, the absence of such a cell should eliminate the pulsations. For a sufficiently high forced concurrent air speed in either μg or $1g$, the main body of the flame will extend downstream of the flame leading edge at the liquid surface. This will affect the preheating distance and could lead to more rapid spread. On the other hand the transport of combustion products ahead of the μg flame could lead to extinction of the flame (as has been seen in some recent Shuttle experiments of flame spread across solid fuels). These open questions are some of the further motivations behind the present work.

The set of three experiments in longer, deeper trays was approved initially for conduct in a sounding rocket, rather than a drop tower, because of the μg test time required to fill the tray with fuel, to reach quiescence in the liquid, and for the flame to spread, and finally because of the volume required by the diagnostic instrumentation. Notably, these were the first μg experiments which enabled an examination of flame spread across pools deep enough for buoyancy in the liquid phase to play a role in $1g$. Comparative tests were conducted in $1g$ in the same hardware.

The experimental results regarding spread and extinction in microgravity were as follows:

- at 30 cm/s opposed air flow, the flame spreads slowly and steadily.
- at 20 cm/s, the same occurs but the flame spreads much more slowly.
- at 10 cm/s, the flame initially spread slowly, weakens as it spreads, and then flashes in a near-extinction behavior.
- at 5 cm/s, the flame flashes part way across the pool and then extinguishes. [This last test was actually a second burn following the 20 cm/s burn.]

These led to the following conclusions:

1. Even with forced air velocities of the same order of magnitude as that induced naturally by buoyancy in normal gravity, the μg flame behavior is completely different (based on the sounding rocket experiment as well as supporting 5.2 s drop tests). Whereas $1g$ flames are soot-producing, and pulsate and spread rapidly, the μg flames are free of soot and spread steadily and slowly.
2. Because of slow propagation speeds in a lower temperature range (one in which a forced air flow is required to sustain flame spread in μg), the observed uniform spread behavior in μg is unrelated to the classical $1g$ uniform spread regime.
3. In μg , a liquid-phase vortex travels steadily with the flame, extends the preheat distance much farther ahead of the flame, carries warm liquid deeper into the pool and has higher rotational velocities than in normal gravity. The center of the vortex is also deeper in μg than in $1g$. This implies that liquid-phase buoyancy serves to stratify the temperature field in $1g$; its absence in μg contributes to the very different liquid surface temperature, flow field and probably the observed flame spread character.

4. Infrared thermography revealed heretofore unobserved surface side-flow phenomena we have labeled "twinning" in 1g and asymmetrical structures far ahead of the flame in μg . These cannot be predicted from the observed flame shape; in fact, the flame shape, which is relatively flat across the tray width in both cases, is a poor indicator of the dimensionality of the flame spread problem.

5. The use of thermal methods, based on refractive index, is misleading in inferring the velocity field ahead of and under the spreading flame. Similarly, the use of an isolated point measurement to determine preheat lengths is misleading because the preheat distance changes throughout the pulsation cycle.

6. The state-of-the-art model's predictions were qualitatively confirmed in regard to gravitational effects on flame shape, trailing flame stand-off distance, flame extinction in μg when there is no opposed air flow, and fuel consumption rate. Agreement between experiment and model is found in the flame spread character and rate in μg when the hot gas expansion is artificially set to zero. The reasons for this are speculated to be as follows: the model is two-dimensional and cannot account for the effects of a finite flame width or the sidewall losses associated with the tray. One consequence of this difference is that hot gas expansion in the model is inherently constrained to the vertical and longitudinal directions. In general, however, hot gas expansion can occur in all directions. Hence gas expansion toward the sides could decrease the effects of hot gas expansion in the direction of flame spread that are predicted by a two-dimensional model. This decrease might be more appreciable in our microgravity experiments (and other μg flame spread studies presently underway) because there is no lateral air inflow driven by buoyancy that would tend to cancel the sideways expansion.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	5	BS Degrees:	5
MS Students:	1	MS Degrees:	1
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 2/91 EXPIRATION: 9/00

PROJECT IDENTIFICATION: 962-22-05-07

NASA CONTRACT NO.: NCC3-121

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Schiller, D.N., Ross, H.D. and Sirignano, W.A. Computational Analysis of flame spread across alcohol pools. Comb. Sci. Tech., (1996).

NASA Tech Briefs

Miller, F.J., Vickerman, M., and Ross, H.D. Video-based, colorized particle image flow visualization. NASA Tech Brief, (1996).

Books

Sirignano, W.A. and Schiller, D.N. "Mechanisms of Flame Spread Across Condensed-Phase Fuels," to appear in "Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman." Edited by: Sawyer, R.F. and Dryer, F.L. Gordon and Breach Publishers, Inc., 1996.

Presentations

Ross, H.D. and Miller, F.J. "Detailed experiments of flame spread across deep butanol pools." 26th International Symposium on Combustion, The Combustion Institute, Naples, Italy, 1996.

Schiller, D.N. and Sirignano, W.A. "Opposed-flow flame spread across n-propanol pools." 26th International Symposium on Combustion, the Combustion Institute, Naples, Italy, 1996.

Presentation Schiller, D.N. and Sirignano, W.A. "Opposed-flow flame spread across n-butanol." 34th AIAA Aerospace Sciences Meeting, Reno, NV, 1996. Paper No. 96-0216.

Combustion Experiments in Reduced Gravity with Two-Component Miscible Droplets

PRINCIPAL INVESTIGATOR: Prof. Benjamin D. Shaw

University of California, Davis

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to study the combustion of bi-component miscible droplets in reduced-gravity environments so that spherical symmetry is strongly promoted. Of particular interest is the burning rate (droplet history), the time to flame contraction, potential microexplosions and the sooting behavior of the droplets. The experiments use liquid mixtures selected to display influences of large component volatility differences and liquid species diffusion on combustion phenomena.

Task Description:

The program is both experimental and theoretical in nature. The experiments will be conducted in ground-based facilities (drop towers and aircraft), and space-based platforms. This program is a continuation of on-going work and will use an existing drop-tower experimental apparatus. Bi-component droplets will be dispensed, deployed and ignited in reduced gravity. The droplet regression history will be measured by backlighting the droplet. An orthogonal view of the flame provides the flame history. This same approach will be used in proposed aircraft experiments. The ground-based experiments will be limited to smaller droplets.

The space-based experiment will use the Droplet Combustion Experiment hardware to examine the combustion history of larger droplets with correspondingly large time and length scales. The flame and droplet imaging systems will remain identical to the current DCE design.

Finally, theoretical and numerical studies will be used to model the combustion of the droplets in reduced gravity. The liquid phase transport processes will be of particular interest. The influence of surface tension driven flows on the liquid phase transport will also be studied.

Task Significance:

The proposed research will extend the current work on combustion of pure liquid fuels to mixtures of pure fuels, which more closely approximate practical fuels. Thus, this program should lead to a better understanding of the combustion of practical liquid fuels.

Progress During FY 1996:

A series of droplet combustion experiments were performed in the 2.2 Second Drop Tower. Flow visualization, and temperature and soot measurements, were performed on single droplets. The data is currently being analyzed, but the analysis has proven to be labor intensive because each film must be viewed many times to make sure that the correct particles are followed when making velocity measurements in the frame-by-frame analysis. During any particular time period, there is a range of particle velocities (which are 2-dimensional velocity measurements) that are observable. The lowest particle velocities are typically a few mm/s, while the maximum particle velocities can be substantially higher. Results from methanol/dodecanol droplets indicate that maximum particle velocities can be as high as (roughly) 100 mm/s, depending on where in the combustion history the measurement is taken. Maximum particle velocities drop to about 20 mm/s just after ignition, grow to values of about 100 mm/s, and the drop again to values of about 20 mm/s after the onset of the flame contraction.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 5/96 EXPIRATION: 4/01

PROJECT IDENTIFICATION: 963-15-OK-0

NASA CONTRACT NO.: NCC3-245

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Aharon, I., Shaw, B.D., Gage, J.W., Jenkins, A.J., and Kahoe, T.K., "Combustion of alcohol mixture droplets in reduced gravity." *Combustion Science and Technology*, (1996).

Presentations

Aharon, I., Shaw, B.D., Gage, J.W., Jenkins, A.J., and Kahoe, T.K., "Combustion of alcohol mixture droplets in reduced gravity." presented at the 1995 Fall Meeting of the Western States Section of the Combustion Institute, paper WSS 95F-228, Stanford, CA., 1995.

Haggard, J.B., Dryer, F.L., Nayagam, V., Shaw, B.D., and Williams, F.A., "Droplet combustion experiments in spacelab." Twenty-Sixth Symposium (International) on Combustion, Naples, Italy, 1996.

Haggard, J.B., Dryer, F.L., Nayagam, V., Shaw, B.D., and Williams, F.A., "Droplet combustion experiments in spacelab." Twenty-Sixth Symposium (International) on Combustion / The Combustion Institute, 1996.

Combustion of Solid Fuel in Very Low Speed Oxygen Streams

PRINCIPAL INVESTIGATOR: Prof. James S. Tien

Case Western Reserve University

CO-INVESTIGATORS:

Sacksteder, K.R.

NASA Lewis Research Center (LeRC)

Ferkul, P.V.

Analex Corporation

Task Objective:

The objectives are to:

1. Enhance the understanding of flame spreading above solid-fuel surfaces through a systematic investigation in the low-speed, forced and buoyant flow regimes.
2. Determine the mechanisms that induce flammability limits of flames over solid surfaces in low-speed flows.
3. Resolve the structure of flames spreading in low-speed flows through a characterization of the velocity, temperature and selected-species fields in their vicinity.

Task Description:

This task consists of the development and flight of a space-based experiment, the continued pursuit of ground-based results in drop towers and aircraft experiments, and the continued development of a comprehensive predictive model of concurrent-flow flame spreading.

The flight experiment is to be accomplished in three phases. An experiment to be conducted in a Glovebox Facility is to provide insight into global flame characteristics of thin and thick fuels. In the second phase, thin fuels are to be burned as they are dispensed from a continuous supply in such a way that the flame is fixed in space relative to the test apparatus. In this way, detailed diagnostic measurements are greatly simplified and transient flame behavior can be observed as the test conditions are slowly varied. In the third phase thick fuels will be burned to address the effect of transverse heat conduction into the fuel, yet with flames spreading slowly enough that the same diagnostic measurements can be made.

The ground-based experimental program consists of observations of flame spreading in partial gravity environments (first attempted as part of this program), the ignition behavior of flames over thin and thick solid fuels in microgravity forced flows, and the implementation of temperature, velocity and species concentration measurement systems.

The model development consists of integrating a fully elliptical fluid mechanics formulation with surface and gas phase radiative interactions in a transient model that attempts to predict the behavior of the selected experimental test fuels in concurrent-flow burning.

Task Significance:

In normal gravity, buoyant air motion in flames is at least 20 to 30 cm/sec. Flame spreading mechanisms that are present only in lower flow velocities, such as spacecraft air-ventilation currents, cannot, therefore, be studied in normal gravity. This research seeks to contribute to fundamental combustion science, and to improve the basis for engineering improved spacecraft fire safety.

Progress During FY 1996:

A device for evaluating the proposed technology for the flight experiment was flight tested aboard the NASA DC-9 reduced gravity aircraft. This device, named the Solid Fuel Delivery System or SFDS, consists of a low-speed wind tunnel enclosed around a spooled strip of thin solid fuel. The fuel is fed into the flow duct under the control of an automated system that detects the leading edge of the fuel as it burns away such that the burnout front of the fuel is kept at a fixed location in the duct. The flame surrounding the fuel is thereby held stationary in the duct, facilitating the probing of the flame with various candidate diagnostic systems.

In flight tests aboard the KC-135 and the DC-9, the SFDS demonstrated improved performance of the continuous fuel supply concept in low-speed purely forced concurrent flows. A new ignition system with a retractable, reusable ignitor was successfully tested aboard the aircraft. Earlier difficulties of collecting and spooling unburnt or partially burnt fuel was resolved with some simple mechanical guides which performed well during aircraft tests. Finally, a programmable traversing thermocouple rake was implemented and tested successfully aboard the aircraft.

2. The Forced Flow Flamespreading Test (FFFT) glovebox experiment was launched aboard the Russian MIR Space Station Priroda Module. The experiment was conducted during NASA/MIR increment 2 by US Astronaut Shannon Lucid. This flight opportunity was used to examine thickness effects on concurrent flow flame spreading over flat cellulosic fuel samples and for some additional tests examining the flow velocity effects on flame spreading over cylindrical polyethylene fuel. The FFFT/MIR hardware was returned from MIR aboard the Space Shuttle as part of STS-79.

The original version of the FFFT experiment was flown aboard the Space Shuttle during the USMP-3 mission on STS-75. These tests examined flow velocity effects on flames spreading over flat cellulosic fuels in different speed concurrent flows, and over cylindrical, heated cellulosic samples. The experiments were completed successfully and have provided unique new data that is being compared to the numerical model developed as part of the SIBAL project. Valuable practical insight was gained from the FFFT/Shuttle experiment for the preparation of the Science Concepts Review of the SIBAL project relevant to requirements for sample length and the interference effect of thermocouples in spreading flames in low speed flows.

3. Following the completion last year of the PhD dissertation of Dr. Ching-Biau Jiang's dissertation at Case Western Reserve University, his model was extended to consider purely buoyant flows, provided predictions of quenching in reduced, but non-zero, gravity levels, which can only be concluded in the presence of radiative losses from the flame. These results, including the effects of gas phase radiative effects were presented to the IAF conference in October, and at the 26th International Combustion Symposium.

4. The numerical model developed for the SIBAL project was modified to account for the hydrodynamic effects of the finite flow duct required for the SIBAL flight experiment. With the duct walls present, the predicted flames are forced closer to the fuel surface by the boundary layer growth, increasing heat transfer to the surface and increasing flame spread rates and fuel burning rates. A Master's Thesis is in progress concerning this work.

5. The Science Concepts Review (SCR) of the SIBAL project was completed successfully, and the authority to proceed to the Requirements Definition Review was granted. The review committee praised the efforts of the SIBAL science and engineering team and suggested that the test matrix for the SIBAL project be expanded to include pressure (and other) effects, and that the SIBAL hardware concept be expanded into a facility class in order to accommodate likely future users.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	2	MS Degrees:	5
PhD Students:	1	PhD Degrees:	3

TASK INITIATION: 2/94 EXPIRATION: 2/99

PROJECT IDENTIFICATION: 962-22-05-40

NASA CONTRACT NO.: NAG3-104

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

T'ien, J.S., Sacksteder, K.R., and Ferkul, P.V.. Solid inflammability boundary at low speed. Science Requirements Document, (June 1996).

Presentations

Jiang, C-B, T'ien, J.S, "Upward flame spread over a thin solid in reduced gravity: model calculations with flame radiation." presented at the 46th International Astronautical Federation Congress, Oslo Norway, October 1995.

Jiang, C-B, T'ien, J.S, and Shih, H-Y, "Model calculation of steady upward flame spread over a thin solid in reduced gravity." Twenty-Sixth Symposium (International) on Combustion, Naples Italy, July 1996.

Jiang, C-B, T'ien, J.S., and Shih, H-Y, "A numerical study of flame radiation effect of forced concurrent-flow flame spread over a solid using discrete ordinates method." presented to the Sixth International Conference on Numerical Combustion, New Orleans, March 1996.

Jiang, Ching-Biau, T'ien, J.S. and Shih, Hsin-Yi "Model calculation of steady upward flame spread over a thin solid in reduced gravity." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28-August 2, 1996.

Droplet Combustion Experiment

PRINCIPAL INVESTIGATOR: Prof. Forman A. Williams

University of California, San Diego

CO-INVESTIGATORS:

Dryer, F.L.

Princeton University

Task Objective:

The objective of this collaboration is to provide scientific support for fundamental, single component, isolated (free and tethered) droplet burning experiments to be performed on board space platforms. The specific objectives of these studies are to provide fundamental results which impact fire safety issues in low gravity environments and to advance the scientific understanding of droplet burning/flame/extinction dynamics over characteristic times which can not be studied in ground based configurations. Engineering and design support functions contribute to: developing and refining methods to perform isolated droplet combustion experiments in general; determining and testing methods to acquire appropriate experimental observations; developing and evaluating methods for presenting and analyzing the collected data. Experimental support functions include: theoretical analyses to define appropriate experimental conditions and to analyze the experimental results obtained; bench scale and drop tower experiments to test and verify methodologies to be applied in the space-based experiments.

Task Description:

The objectives are pursued experimentally in ground-based bench facilities at the respective institutions and NASA Lewis, as well as in the 2.2 Second and 5 Second Drop Towers located at NASA-Lewis. Studies include isolated, filament-suspended and free droplet studies in bench scale facilities (200 to 1000 micro-meter diameter), 2.2 Second Drop Tower experiments in tethered and free droplet modes (1000 to 1500 micro-meter diameter), and 5 Second Drop Tower experiments in tethered and free droplet modes. Theoretical analyses based on asymptotic methods are pursued at the University of California San Diego, while uni-dimensional (sphero-symmetric) and two-dimensional axi-symmetric numerical computations are pursued at Princeton. The fuels of interest to this work include: normal-heptane, normal decane, methanol, and methanol-water mixtures.

Experiments are performed at varying ambient pressures, oxygen contents, and with varying diluent species to develop an experimental data base over parameter ranges which can be studied in the available test times in each facility. Flight experiments are required because of the very long test times and low gravity conditions required for significant portions of the work. Data typically obtained include back-lighted images of the droplet, and direct light images of the flame structure as functions of the experimental test time. Data are acquired film as well as through video imaging (inclusive of intensified imaging methods to obtain direct light intensity distributions over specific wavelengths) as a means of producing quantitative comparisons of flame image with model predictions. Image data are processed using high precision methods to obtain droplet diameter history, flame structure history, and extinction diameter. These parameters are then directly compared with theoretical predictions. In ground-based experiments, supplemental experimental measurements such as integrated droplet chemical composition history, and direct light imaging measurements at several wavelength ranges can be obtained for comparison with model predictions. Data obtained in ground-based experiments complement that which can be obtained in flight experiments in that the characteristic times of the former extend from (with some overlap) to times considerably shorter and with droplet diameters much smaller than can be studied in the latter.

Task Significance:

The overall purpose of the research is to achieve fundamental advances in the science of droplet combustion, which is central to a number of energy-producing devices and systems. In particular, unsteady liquid and gas phenomenon, and extinction chemistry of normal alkanes and simple alcohols are investigated.

Progress During FY 1996:**Studies at the University of California-San Diego**

Analytical modeling on the structure and extinction of quasi-steady, spherically symmetric diffusion flames around methanol and n-heptane droplets continued during this reporting period. The issue of combustion generated water dissolution into the methanol fuel droplet was investigated using asymptotic techniques. The results are shown to

agree qualitatively with the recent flight experimental results (USML-2 Glovebox experiment - Fiber Supported Droplet Combustion (FSDC) experiment). A revised chemical kinetic scheme for n-heptane fuel combustion is currently under development. This improved kinetic scheme should produce better agreement with the drop-tower results for n-heptane droplets burning in Oxygen/Helium environments and provide better burning time estimates for the up coming flight experiment.

The FSDC Glovebox (USML-2) experimental results for methanol, methanol/water and methanol/dodecanol droplets were analyzed in collaboration with NASA Lewis personnel. The results show that the data on the combustion of large fuel droplets are valuable for testing droplet-burning theories.

Studies at Princeton University

In addition to supporting the engineering development of the flight experiment for DCE, and experimental studies in the 2.2 second drop tower (see below), efforts have further advanced the computational tools and sub-models for numerically predicting the combustion of methanol and normal heptane droplets. Progress in each of these areas is summarized below.

Drop-Tower Studies

In collaboration with NASA Lewis performed 2.2 second drop-tower studies at NASA-Lewis (using methanol and methanol-water as fuels) to support science development for both of the FSDC flights and the proposed second flight of DCE. These studies developed extensive data on burning rate and on chemiluminescent flame characteristics as functions of initial conditions (drop diameter, initial oxygen mole fraction, and environment pressure) and burning time. The work also provided a comprehensive data-base on criteria for hot wire ignition of methanol and methanol/water droplets under various initial conditions to support hardware development and verification for DCE. In collaboration with the engineering team developing and testing hardware for DCE in the 5.5 ZGF facility, drop tower data for n-heptane combustion, particularly chemiluminescent flame data, were analyzed both experimentally and numerically, and results were compared with those found for methanol droplets. These results show that water dissolution and accumulation are substantially affected by internal liquid phase motions. Also, it was found that radiative effects are small for methanol droplet burning at diameters below about 1.5 mm. Further more, chemiluminescent flame imaging, along with detailed kinetic modeling which includes chemiluminescent species, was shown to be a quantitative approach to comparing flame data with modeling results. This finding establishes that flame structure studies can be performed with methods which are much less complex than laser-based species measurement techniques such as CARS or LIF. The chemiluminescent imaging methods developed as part of DCE were thus established to be adequate for meeting the science requirements for this experiment

FSDC I

Princeton participated in FSDC I by defining test matrices for methanol and methanol/water droplet experiments through numerical calculations, by participating in training exercises for operation of the experiment from the payload operations communications center (POCC), and by participation in the actual flight (STS-73) in late October and early November 1995. A number of successful methanol and methanol/water (10/90%, 20/80%) experiments for initial droplet diameters larger than 3.0 millimeters were performed. Comparing the experimental observations with adiabatic numerical computations the following conclusions are drawn:

1. Water accumulation inside the liquid droplet causes a substantial increase in droplet extinction diameter with increases in initial droplet diameter, in agreement with the ground observations and numerical calculations.
2. Spectral (molecular) radiative exchange apparently results in non-adiabatic combustion conditions for the large droplet diameters studied (greater than 3.0 mm) in the FSDC I experiments. Thus large diameter droplet studies which are only possible in space conditions apparently offer a unique opportunity to study radiative effects on combustion in general and droplet burning in particular. Subsequent numerical model development and computations which includes spectral radiative effects strongly supports this point. The modified model closely predicts the extinction diameter data obtained for methanol droplets (including the non-linear dependence of the extinction diameter on initial diameter), as well as the burning rate data experimentally observed for large methanol and methanol/water droplets. Continuing analyses of the entire FSDC I data further substantiates these earlier results.

Sphero-symmetric Numerical Modeling Advances

The initial time-dependent numerical model developed as part of this has been further updated in terms of kinetic and physical property data to include: a new comprehensive model for methanol which considers pressure-dependent reaction effects a new semi-empirical model for n-heptane combustion, the chemical kinetic mechanism of for n-heptane combustion, inclusive of modifications to predict n-heptane/n-hexadecane combustion, and binary liquid properties (including methanol/water and n-heptane/n-hexadecane mixtures). In addition, a major modification of the model has been performed to include spectral radiative transfer effects for the major combustion products, CO, CO₂, and H₂O. The mean-plank absorption coefficient calculations performed in the model are both spatially and time dependent, and fully coupled to detailed chemical kinetics and transport. Initial results from the revised suggested that radiative effects are substantial in the large diameter methanol and methanol/water droplet combustion experiments conducted on FSDC I. Further modifications of the model to eventually include soot shell formation, and continuum radiation effects for sooting droplet combustion have been initiated.

Axi-Symmetric Modeling Efforts

A major effort during the reporting period has been devoted to further developing and demonstrating a two-dimensional, axi-symmetric, time-dependent, reacting flow numerical approach based on spectral element methods. The method is very general and should provide new insights to a number of symmetrical, reacting flow phenomena involving convection. As developed thus far, the model is capable of using semi-detailed kinetics considering up to about sixteen species and includes a multi-species diffusion model to describe the transport processes. The incorporation of these detailed sub-model components enables the numerical model to simulate the transient phenomena inclusive of gas phase motions and ignition.

The utility of the model was demonstrated by solving two different reacting flow problems, a carbon particle burning in a convective environment, and a porous sphere diffusion flame in a convecting environment. The simulations performed reveal the effects of low Reynolds number flow on the ignition and flame structure development of a spherical non-premixed CO/air flame and on the gasification behavior of a small (200 μ m in diameter) Spherocarb (model-carbon) particle. At a Reynolds number of unity, the steady-state non-premixed CO/air flame is almost spherically symmetric; however, during the ignition process, deviations from spherical-symmetry are significant. As for the spherocarb particle simulation, the burning mode of a small carbon particle is sensitive to the Reynolds number (in the range $0 < Re < 10$). It changes from a fast burning mode at $Re=1$ (or less), with the presence of a reactive boundary layer surrounding the particle, to a heterogeneous kinetics controlled, slow burning mode at $Re=10$ with non-trivial gas-phase chemistry in the wake.

The present model has not yet included the complication of coupling the liquid and gas phase flow fields at the droplet interface. Liquid phase coupling with the gas phase flow field is presently being incorporated into the numerical model.

Program Reviews

During this reporting period a successful Pre-Ship Review for the Droplet Combustion Experiment (DCE) was completed in collaboration with the NASA personnel. The DCE hardware was shipped to KSC and integrated into the Spacelab ready for the MSL-1 mission.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	5

TASK INITIATION: 3/91 EXPIRATION: 3/00

PROJECT IDENTIFICATION: 963-22-05-08

NASA CONTRACT NO.: NCC3-407

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Held, T.J., Marchese, A.J., and Dryer, F.L., A semi-empirical reaction mechanism for -n-heptane oxidation and pyrolysis. *Combustion Science and Technology*, (April, 1996).

Lee, J.C., Tomboulides, A.G., Orszag, S.A., Yetter, R.A., and Dryer, F.L. Integrated asymptotic analysis and numerical simulation of laminar flow reactors. *Combustion Science and Technology*, (July 17, 1996).

Lee, J.C., Yetter, R.A., and Dryer, F. L., Numerical simulation of laser ignition of an isolated carbon particle in quiescent environment. *Combustion and Flame*, 105, 591 (1996).

Marchese, A.J., and Dryer, F.L., Effect of liquid mass transport on the combustion and extinction of Bi component liquid droplets of methanol and water. *Combustion and Flame*, 105, 104 (1996).

Marchese A.J., and Dryer, F.L., The effect of non-luminous thermal radiation in microgravity droplet combustion. *Combustion Science and Technology*, (July 18, 1996).

Marchese, A.J., and Dryer, F.L., The effect of non-luminous thermal radiation in microgravity droplet combustion. *Mechanical and Aerospace Engineering*, 2074, (1996).

Presentations

Dietrich, D.L., Haggard, J.B. Jr., Dryer, F.L., Nayagam, V., Shaw, B.D., and Williams, F.A. "Droplet combustion experiments in Spacelab." Twenty Sixth International Symposium, Naples, Italy, July 22-August 2, 1996.

Lee, C.J., Tomboulides, A.G., Orszag, S.A., Yetter, R.A., and Dryer, F.L., "A transient two-dimensional chemically reactive flow model: Fuel particle combustion in a non-quiescent environment." Twenty Sixth International Symposium, Naples, Italy, July 22-August 2, 1996.

Lee, J.C., "Simulations of two dimensional chemically reactive flow." Ph.D. Thesis, Mechanical and Aerospace Engineering Dept., Princeton University, Princeton, NJ, MAE Report No. 2063-T, June, 1996.

Lee, J.C., Tomboulides, A.G., Orszag, S.A., Yetter, R.A., and Dryer, F.L., "Asymptotic and numerical modeling of laminar flow reactors." Third Workshop on Modeling of Chemical Reaction Systems, Heidelberg, Germany, July 24-26, 1996.

Lee, J.C., Tomboulides, A.G., Orszag, S.A., Yetter, R.A., and Dryer, F.L., "Asymptotic and numerical modeling of laminar flow reactors." Poster presentation, Twenty-Sixth International Symposium on Combustion, Poster No. 04-84, Naples, Italy, July 22-August 2, 1996.

Marchese, A.J., "Combustion of single and bicoponent liquid droplets: Detailed kinetic modeling and microgravity experiments." Ph.D. Thesis, Mechanical and Aerospace Engineering Dept., Princeton University, Princeton, NJ, MAE Report No. 2081-T, 1996.

Marchese, A.J. and Dryer, F.L., "The effect of non-luminous gas phase radiation on the combustion of large droplets in microgravity." Twenty-Sixth International Symposium on Combustion, Naples, Italy, Poster No. 5-083, July 22-August 2, 1996.

Marchese, A.J., Dryer, F.L., Nayagam, V., "Microgravity combustion of methanol and methanol/water droplets: Drop tower experiments and model predictions." Twenty Sixth International Symposium, Naples, Italy, July 28-August 2, 1996.

Marchese, A.J., Dryer, F.L., Nayagam, V., and Colantonio, R., "Hydroxyl radical chemiluminescence imaging and the structure of microgravity droplet flames." Twenty Sixth International Symposium, Naples, Italy, July 28-August 2, 1996.

Zhang, B.L. and Williams, F.A., "Theoretical studies of methanol droplet combustion based on results from the Shuttle spacelab during the USML-2 mission." 47th International Astronautical Congress. IAF-96-J.3.12, Beijing, 1996.

Zhang, B.L. and Williams, F.A., "Simplified analyses of methanol droplet combustion for comparison with microgravity experimental results." 34th Aerospace Sciences Meeting and Exhibit, AIAA-96-0263, Reno, 1996.

Zhang, B.L., and Williams, F.A., "Alcohol droplet combustion." 46th International Astronautical Congress, IAF-95-J.1.05, Oslo, Norway, 1995; *Acta Astronautica*, in press, 1996.

Surface Controlled Phenomena

PRINCIPAL INVESTIGATOR: Prof. Robert E. Apfel

Yale University

CO-INVESTIGATORS:

Holt, R.G.
Tian, Y.

Jet Propulsion Laboratory (JPL)
Yale University

Task Objective:

The goals of this research are to investigate the rheological properties of surfactant-bearing liquid drops. By comparing experimental results in the ideal environment of the Spacelab to our theory for spherical equilibrium drops, we can validate the model. We can then synthesize a generic theory which can handle arbitrary acoustic fields and static deformations, in order to have a technique for studying static and dynamic surface properties for surfactant-bearing drops which can be successfully applied in 1-g experiments.

Task Description:

Single liquid drops are introduced into the center node of an acoustic standing wave in DPM's Near-Ambient Chamber. They are allowed to reach quiescent equilibrium. Then, shape oscillations about either a spherical or a spheroidal equilibrium shape are excited - either by a momentary increase and release of the z-axis acoustic pressure or by a periodic modulation of that pressure. The resulting oscillations are recorded on video tape and ciné film for later analysis.

Three sample materials will be investigated on USML-2: triply distilled water, water with small amounts of Triton X-100 or bovine serum albumin at five different concentrations. The additives provide contrasting time scales: Triton X-100 is a nonionic fast-sorbing surfactant while BSA is sorption-inhibited. A range of drop sizes from 4 to 12 cc will be investigated for each of concentration.

Task Significance:

The flight experimental data will be used to validate the theory which describes drop shape-oscillations as a function of various surface parameters. These parameters will be obtained in microgravity from drops oscillating about a spherical equilibrium shape as well as about an acoustically induced oblate shape. By comparing the differences in the natural frequency and damping constant for these oscillations, the theory and experimental techniques can be used to perform measurements of the surface properties on the ground. Theoretical development and ground-based experiments to support the microgravity work are also performed.

Progress During FY 1996:

In FY 96, we have carried out a series of experiments on STS 73 utilizing the Drop Physics Module (DPM-2) as part of USML-2. Our experiments have primarily focused on the determination of the rheological properties of surfactant bearing drops by examining the dynamics of drops after they have deformed (using acoustical techniques). Our experiments have enabled us to observe: 1) small amplitude oscillations about a spherical shape, 2) small oscillations about a deformed shape, 3) static deformations up to an aspect ratio of 3.5, and 4) superoscillations of greatly deformed drops. We considered pure water and aqueous solutions of two surfactant (triton X100 and BSA) in various concentrations, up to twice the critical micelle concentration. The quality of the data was very significantly better than that achieved on USML-1 (in 1992). We are analyzing some 82 drop sequences from the video tape and cine record. We have also performed extensive analysis using the boundary integral method, and we have seen excellent correspondence between theory and experiment, permitting us to extract dynamic surface properties, such as surface tension, Gibbs Elasticity, and surface viscosity. The data can be interpreted by comparing with ground based data from our lab with much small drops, and by putting it in the context of a theoretical formalism also developed in our laboratory. Three manuscripts have been submitted for publication, and three have been published in FY96.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	3	BS Degrees:	3
MS Students:	2	MS Degrees:	0
PhD Students:	3	PhD Degrees:	1

TASK INITIATION: 2/90 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 963-24-04-03

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Shi, W. and Apfel, R. Deformation and position of acoustically levitated liquid. J. Acoust. Soc. Am, vol 94, 1977-1984 (1966).

Shi, W.T., Apfel, R. E. and Holt, R. G. The instabilities of liquid drops in sound field. Phys. of Fluids, Vol 7, no. 11, 2601-2607 (1995).

Tian, Y., Holt, R.G., and Apfel, R. E. Investigations of liquid surface rheology of surfactant by droplet shape oscillations. Phys. of Fluids, 7 (12), 2938-2949 (1996).

Two-Phase Gas-Liquid Flows in Microgravity: Experimental and Theoretical Investigation of the Annular Flow

PRINCIPAL INVESTIGATOR: Prof. Vemuri Balakotaiah

University of Houston

CO-INVESTIGATORS:

Jayawardena, S.

University of Houston

Task Objective:

Two phase gas-liquid and vapor-liquid flows with heat transfer occur in a variety of process equipment such as petroleum production facilities, condensers and reboilers, gas-liquid reactors, trickle-bed contactors, wetted wall absorbers, falling film reactors, power systems and core cooling of nuclear power plant during emergency operation. In addition to these normal gravity commercial applications, two-phase flows are expected to occur in a variety of future space operations such as active thermal control systems, power cycles, propulsion devices and storage and transfer of cryogenic fluids. In order to design these systems with greater efficiency and minimum cost, a fundamental understanding of the transport processes occurring in normal and microgravity two-phase flows is needed.

For conditions of technological interest, there are three major types of flow regimes observed for gas-liquid flows in pipes. At low gas flow rates, a "bubbly flow" pattern in which, small gas bubbles are uniformly distributed in the liquid, is obtained. Increasing the gas flow rate leads to "slug flow". This flow pattern is characterized by large bullet shaped gas bubbles separated by liquid slugs. Increasing the gas flow rate further leads to the annular flow regime. In microgravity, annular flows are obtained for a wider range of gas and liquid flow rates. Experiments have shown that in the annular flow regime, the waves appearing on the liquid film have a profound influence on the transfer of heat and momentum (or pressure drop) in these systems. Neglecting the wavy nature of the film can seriously underestimate the transfer rates.

The main objective of this work is to understand through a combined program of experimental and modeling studies, two-phase gas-liquid flows in pipes under normal as well as microgravity conditions. The specific objectives of this project are: (i) development and testing of predictive models for fully developed annular flows under normal and microgravity conditions (ii) measurement and analysis of data on the statistics of wavy films (film thickness, wave velocities, power spectrum, etc.) and comparison with models (iii) modeling studies on the scale-up of two-phase flows to predict flow regimes and transitions at zero-gravity and validation with data (iv) extension of models to predict wall shear stress (pressure drop) and heat and mass transfer coefficients for annular two-phase flows.

Task Description:

The experimental part of the project has three tasks:

1. Ground based experimental studies on the air-water annular flows using the two-phase test rig at LeRC.
2. Development and testing of a ground based two-phase flow test rig for the refrigerant R-134a.
3. Development of the flight based flow loop and sensors for measuring film thickness, wall shear stress and wave velocities in microgravity annular two-phase flows.

The modeling studies will be done in parallel. The main task is to develop simplified predictive models (based on valid simplifications of the Navier-Stokes equations) to describe the statistics of wavy films at normal as well as microgravity conditions.

Task Significance:

Two-phase annular flows occur in many space operations such as active thermal control systems, power cycles, propulsion devices and storage and transfer of cryogenic fluids. In addition, a fundamental understanding of the transport processes occurring in two-phase flows is essential in the design of process equipment in the chemical, petrochemical, pharmaceutical and nuclear industries.

The experimental database obtained here may be used in the design of microgravity two-phase active thermal control systems, development and testing of models and in the fundamental understanding of normal and microgravity two-phase flows.

The predictive models will guide the experiments and minimize the number of different experiments to be done.

Progress During FY 1996:

Modeling:

1. All the existing data on two-phase flows in microgravity has been analyzed and a new (and the first comprehensive) flow pattern map has been developed.
2. Models previously developed for free falling films have been extended to include co- and counter-current flow of gas. The analysis of these models as well as the extension to microgravity conditions is in progress.

Experimental:

1. Design of a ground based R-134a flow loop is complete.
2. Developed sensors for measurement of void fraction and wall shear stress specific to R-134a.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 963-25-OH

NASA CONTRACT NO.: NAG3-184

RESPONSIBLE CENTER: LeRC

Critical Viscosity of Xenon

PRINCIPAL INVESTIGATOR: Dr. Robert F. Berg

National Institute of Standards and Technology

CO-INVESTIGATORS:

Moldover, M.R.

National Institute of Standards and Technology (NIST)

Task Objective:

The objective of the experiment is to produce archival viscosity data on xenon that is closer to its liquid-vapor critical point than is possible in Earth's gravity.

Task Description:

Develop a viscometer whose frequency and shear rate are sufficiently low for accurate measurements near xenon's critical point. The viscometer must be insensitive to vibrations which occur in orbit. Its accuracy must be 0.2% or better.

Develop a thermostat whose temperature stability is better than 100 microkelvin per hour and whose temperature gradient is less than 0.2 microkelvin over 4 centimeters.

Load and seal a viscometer cell with xenon to within 0.3% of the critical density.

Devise a temperature schedule which is realistic for a Space Shuttle flight and which will produce density differences within the xenon which are no greater than 0.3%.

Operate the flight instrument before, during, and after the flight.

Task Significance:

Near the liquid-vapor critical point, theory predicts a power-law divergence of the viscosity. The inhomogeneity caused by Earth's gravity has always blunted this divergence into only a modest increase. The flight experiment will provide the first direct observation of the divergence of viscosity in a pure fluid. It will test theories for the crossover to the critical region and for the value of the exponent associated with the divergence. Also, in combination with the results from the Critical Fluid Light Scattering Experiment (Zeno), the data will provide a stringent test of dynamic critical phenomena.

Progress During FY 1996:

Performance in 1-g of the NIST viscometer:

We analyzed viscosity measurements made at NIST in a flight-qualified cell following a flight-like temperature timeline. The apparent viscosity values have a 1s statistical uncertainty of 0.03%, well within the requirement of 0.2%. Additional measurements demonstrated the viscometer's stability was 0.1% over six months.

The effect of internal waves on the NIST viscometer:

Close to the critical temperature, the 1-g measurements differed from our previous measurements made in a torsion oscillator cup. This difference was attributed to the excitation of internal waves, an effect which will be absent in microgravity. To support this attribution, we carefully scrutinized the effects of internal waves on the oscillator's transfer function. First, in a collaboration with applied mathematicians at NIST, we proved the existence of internal waves in the viscometer by studying their frequency spectrum. Second, we demonstrated that the deviations of the measured transfer function from the zero-gravity model of the transfer function required the presence of a stratification profile in the xenon.

Measurements of the viscometry electronics' stability:

Initial tests of the flight instrument showed that the viscometry output was unstable, with a time dependence uncorrelated with ambient temperature. The source of this irreproducibility, discovered only after components of the NIST prototype and the flight instrument were systematically interchanged, was traced to a pair of blocking capacitors. After replacement of these (high quality ceramic) capacitors by silver mica capacitors, the viscometry was stable to within 0.1%.

Measurement of the viscometer's vibration susceptibility:

The CVX viscometer's signal-to-noise ratio will be reduced by vibrations, or "g-jitter", typical of the Space Shuttle in orbit. The vibration susceptibility was measured by suspending the flight experiment by a chain, attaching a shaker and an accelerometer, and then taking viscometry data while vibrating the instrument. Random vibrations below 20 micro-g per root hertz had a negligible effect. No resonances of the instrument were noted below 25 hertz. The susceptibility was approximately equal to the model used in the Science Requirements Document and is thus acceptable.

Measurement of the thermostat's temperature stability:

We collaborated in tests of the thermostat's temperature stability. These tests compared four thermometers: (1) the thermistor installed on the cell, (2) a thermistor installed on the surrounding thermostat shell, (3) the viscosity's temperature dependence, and (4) a second, independently-measured thermistor installed temporarily on the cell. Comparison between the first and second thermometers revealed a persistent 3-month drift in the difference of their temperatures. Comparison with the third thermometer revealed the drift was due solely to the cell's thermistor, which was subsequently replaced. In addition to the long-term drift, random short-term variations of as much as 150 microkelvin in 30 hours were observed. The fourth thermometer verified that these short-term variations were actual temperature variations and not thermometry errors, and thus they are acceptable.

Measurement of the thermostat's temperature gradient:

The requirement that temperature differences within the xenon be less than 0.2 microkelvin is unusually stringent. Therefore we collaborated in direct measurements which verified the thermostat's ability to achieve this requirement. We replaced the thick-walled copper sample cell by a thin-walled steel cell whose lower thermal conductance "amplified" the axial temperature difference by a factor of 60. The steel cell contained a pair of thermistors and a thermocouple pile, thus allowing two independent methods to measure the end-to-end temperature difference. The thermostat performed satisfactorily during temperature ramps and during the imposition of external temperature gradients. At zero ramp rate, the temperature difference along the steel cell was 5 microkelvin. This implies that the copper cell's temperature difference will be only 0.08 microkelvin, well within the requirement.

Temperature schedule:

During the flight experiment, viscosity must be measured in the range of temperatures from $T_c + 60$ mK to $T_c + 0.6$ mK without creating large density disturbances near the oscillator. (T_c is the critical temperature.) The thermal diffusivity of xenon vanishes as T_c is approached, while its thermal expansivity diverges. Thus a long-lived density inhomogeneity can be created by changing the sample's temperature too quickly. We used a one-dimensional, finite element model of the sample cell to calculate the effects of temperature changes. The numerical model combined the equation for heat transfer in a compressible fluid with xenon's equation of state. It was checked against two analytical calculations. Additional analytical calculations were used to estimate the inaccuracy caused by the numerical model's geometrical assumptions. The final timeline was shown to meet the requirements of CVX during a nine-day Shuttle mission.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 1/94 EXPIRATION: 1/97

PROJECT IDENTIFICATION: 963-03-0A-19

NASA CONTRACT NO.: C-32014C

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Berg, R.F., Lyell, M.J., McFadden, G.B., and Rehm, R.G., Internal waves in xenon near the critical point. Phys. Fluids, 8, p. 1464 (1996).

Presentations

Berg, R.F., "Internal waves in xenon near the critical point." March meeting of the American Physical Society, St. Louis, MO, March 20, 1996.

Berg, R.F., "Internal waves in CVX." Third Microgravity Fluid Physics Conference, Cleveland, OH, June 14, 1996.

The Dynamics of Disorder-Order Transitions in Hard Sphere Colloidal Dispersions

PRINCIPAL INVESTIGATOR: Prof. Paul M. Chaikin

Princeton University

CO-INVESTIGATORS:

Russell, W.B.
Zhu, J.

Princeton University
Princeton University

Task Objective:

To study the disorder-order transition in a hard sphere colloidal particle system, utilizing laser light scattering to detect (1) viscosity changes as the transition from fluid to crystal to glass occurs, (2) diffusion of particles, (3) nucleation and growth of the crystals and (4) rigidity after the transition is complete.

Task Description:

The approach has focused on simulating low-gravity by fluidizing a bed of specially prepared hard spheres (silica particles with short polymer coatings) with a counterflow of solvent. The counterflow allows an approximation of microgravity. Results of this study are compared with those obtained using the Physics of Hard Spheres Experiment (PHaSE) flight breadboard and the PHaSE flight system (before delivery to the cape) allowing the development of a baseline for the flight samples. The flight samples range in volume fraction from those which will remain as fluids, to those which will exhibit the properties of glass. The in-between phase, where fluid and crystals coexist, is of greatest interest. It is this region where, depending on the volume fraction of PMMA to decalin/tetralin, the formation of large crystallites is expected. Light intensity data from these samples will allow the determination of crystal structure dynamics and rheology.

Task Significance:

The study of crystal formation in the microgravity environment can lead to a greater understanding of how gravity affects the formation of many kinds of colloidal materials. Colloidal materials of some note are semi-conducting materials, liquid crystals, paints and coatings, biofluids, etc. Understanding these complex materials may open the door to new ways of using the materials we have, and possibly lead to the discovery of new valuable materials. The focus of the experiment is to use a material which can exist in multiple phases depending on its concentration in a colloidal suspension. Laser light scattering images will provide structural information about the material as it goes through liquid, ordered crystal, and disordered glass phases.

Progress During FY 1996:

In the Princeton fluidized bed the shear modulus and viscosity of the hard sphere dispersion are detected via Bragg Spectroscopy. When the amplitude of the oscillation is small relative to the inverse of the scattering wave vector, the scattered intensity fluctuates at the same frequency, and the ensemble averaged temporal autocorrelation function of the scattered intensity from the center of the bed indicates the amplitude of the response. The rheological properties are then extracted by modeling the colloidal system as a linear viscoelastic solid.

The scattering intensity pattern at low angles from a crystalline dispersion in the Princeton fluidized bed forms five symmetric rings on each side. The Bragg angles indicate an fcc structure for a fluidized hard sphere crystal, since the ratios of the corresponding scattering wave vectors match all lines for the fcc crystal. However, the intensity of the second Bragg peak is much less than the first, suggesting that some crystal grains may have randomly stacked hexagonal structures which contribute to the intensity of all but the second peak. Thus the structure observed may be a mixture of face-centered-cubic and randomly stacked crystallites. The flight experiment should confirm if the structure is pure fcc or a mixture of fcc and randomly deposited hcp structures.

The samples needed for the flight experiment have been prepared by Princeton and have been integrated into the flight instrument.

The instrument itself has been designed and built. There is an operational breadboard located at Princeton which incorporates many of the functions of the flight hardware. Unfortunately it was not possible to incorporate each

flight function into the PHaSE breadboard. The breadboard was used to develop operational procedures for the flight experiment and to verify software functionality. Baseline data has been obtained on samples which contain the same proportions of PMMA in suspension found in the flight samples. Data from the fluidized bed, the breadboard, and the flight hardware (before delivery to NASA - Kennedy Space Center) have been used to develop a mathematical model which is used to predict colloidal dispersion dynamics.

The PHaSE flight hardware is now being subjected to flight acceptance testing (thermal cycles, mechanical and electronic emissions determination, and random vibration) for flightworthiness determination. During thermal cycling some anomalies were identified which need to be corrected before the hardware is delivered to KSC. One anomaly involved the cooling of the digitizing board which supplied digital images of the Bragg screen during the process of sample crystallization. The board was relocated to another slot in the card cage which allows the circulating fan to cool it more effectively. The same card also had a problem with components which had loosened during thermal cycling. This has been remedied by purchasing a soldered board from the manufacturer. Another anomaly occurred with the motor which turns the carousel which holds the sample cells and positions them for viewing, etc. The motor would intermittently fail to rotate the carousel. It was determined that the shaft was slightly out-of-round and that the pre-load required adjustment. There has been no anomalous event of this type since the adjustments were made. The adjustments did result in a positional error of approximately 0.02 degrees in the reverse directional mode. An operational procedure was written which allows the user to compensate for this error on position the carousel properly.

The flight hardware is presently being tested by the Principal Investigator team in order to confirm it functions as required to satisfy science priorities and requirements, including a full mission simulation. The hardware is scheduled to be shipped to NASA - Kennedy Space Center on Sept. 3, 1996. It will be integrated into an express rack (like the type which will be utilized on the International Space Station) which will be fitted into the Shuttle SpaceLab module. Launch date is scheduled for early April 1997.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 1/96 EXPIRATION: 6/99

PROJECT IDENTIFICATION: 963-24-05-10

NASA CONTRACT NO.: NAG3-176

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Rutgers, M.A., Dunsmuir, J., Russel, W.B., and Chaikin, P.M., Hard sphere equation of state. Science, (1995).

Rutgers, M.A., Russel, W.B., Chaikin, P.M., and Dunsmuir, J.H., Real hard spheres. American Physical Society, vol. 40, no. 1, (1995).

Rutgers, M.A., Xue, J.Z., Herbolzheimer, E., Russel, W.B., and Chaikin, P.M., Crystalline fluidized beds. Physical Review E, 51, 4674 (1995).

Zhu, J.X., Phan, S.E., Russel, W.B., Chaikin, P.M., Absorption of tetralin by PMMA spheres in decalin/tetralin mixture. American Physical Society, vol. 40, no. 1, (1995).

Proceedings

Chaikin, P.M., Zhu, J., Russel, W.B., "Dynamics of disorder-order transitions in hard sphere colloidal dispersions in microgravity." Proceedings of Third Microgravity Fluid Physics Conference, 1996.

Investigations of Mechanisms Associated with Nucleate Boiling under Microgravity Conditions

PRINCIPAL INVESTIGATOR: Dr. Vijay K. Dhir

University of California, Los Angeles

CO-INVESTIGATORS:

Hasan, M.

NASA Lewis Research Center (LeRC)

Task Objective:

In this work a building block type of approach is used so that a basic understanding of the processes that contribute to nucleate boiling heat fluxes under microgravity conditions can be developed. This understanding will lead to development of a mechanistic model for nucleate boiling heat transfer under microgravity conditions. The work is both experimental and analytical/numerical in nature. Experiments are to be performed both at earth gravity as well as low gravity conditions in the DC-9 aircraft and in the ISSF Fluids Combustion Facility. The key processes that will be studied in this work are:

1. Heat transfer to a single bubble including that associated with micro/macro layer evaporation.
2. Bubble merger process and heat transfer to vapor stems supporting a large bubble (may be mushroom type) attached to heater wall.
3. Detachment process of small as well as large mushroom type of bubbles.
4. Flow field induced by bubbles during growth and detachment including that due to Marangoni effect.
5. Heat transfer and flow field for a bubble sliding along a heated wall.

Task Description:

The total effort is divided into five tasks. These tasks are:

Task 1: Fabrication of the Experimental Setup. Under this task, the test section and liquid holding and viewing chambers will be fabricated. Artificial cylinder cavities will be formed on silicon wafers. A single cavity and two or four cavities, with a prescribed spacing and size, will be formed. The desired nucleation wall superheat will be used to determine the size of the mouth of the cavities.

Task 2: Experiments. The basic experiments for flow and temperature field around single and multiple (2 or 4 separated or merged bubbles growing on downward facing or inclined surfaces) will be carried out under normal gravity conditions. The experiments will be conducted at one atmosphere pressure, but liquid subcooling will be varied from 0 to 30°C (PF-50 50) and 70 to 100°C (water). Water and PF-5050 will be used as test liquids.

Task 3: Analytical/Numerical Models. In this task, transient temperature and flow field in vapor and liquid will be determined during growth of a single bubble. Analysis will include the evolution of the vapor-liquid interface and development of microlayer underneath the bubbles. For merged bubbles, detailed calculations of flow and temperature field will be carried out for transient shapes of vapor stems supporting a large bubble and the corresponding evaporation rate. Flow and temperature field for a bubble sliding along a heated wall will also be determined. Microgravity conditions will be simulated and a framework of a numerical tool for prediction of nucleate boiling heat fluxes under microgravity conditions will be developed.

Task 4: Experiments in DC-9 or Lear Jet. To understand bubble growth and detachment behavior of single or large merged bubbles, boiling experiments will be conducted under low gravity (10^{-2} g) conditions of the aircraft. In these experiments, "designed" surfaces will be used. Visual observations and heat transfer data will be taken, but holography will not be used. The apparatus used for laboratory experiments will also be employed for experiments in the aircraft.

Task 5: Experiments in the Space Shuttle. Effort will be devoted for defining a boiling experiment to be conducted on a "designed" surface. The experiment will provide microgravity data on bubble growth and departure. These data are needed for development of a credible model for nucleate boiling heat fluxes under microgravity conditions. The heat transfer data will also be obtained and will be used to validate the models.

Task Significance:

Boiling is known to be a very efficient mode of heat transfer, and as such, it is employed in component cooling and in various energy conversion systems. For space applications boiling is the heat transfer mode of choice, since for a given power rating the size of the components can be significantly reduced. For any space mission, the size, and in turn, the weight of the components play an important role in the economics of the mission.

Applications of boiling heat transfer in space can be found in the areas of thermal management, fluid handling and control, and power systems. For space power systems based on the Rankine cycle (a representative power cycle), key issues that need to be addressed are the magnitude of nucleate boiling heat transfer coefficient and the critical heat flux under low-gravity conditions. Knowledge of nucleate boiling heat transfer coefficient is necessary to determine the overall resistance for transfer of heat from a source to a sink. The critical heat flux represents the upper limit for safe heat removal since for heat fluxes greater than critical heat flux, the surface will be covered with a vapor film which in turn will result in a rapid rise in the temperature or failure of the component.

Understanding and quantification of boiling heat fluxes at low-gravity conditions are also important for other space power systems such as thermionic reactors operating under transient conditions. Design of on-orbit storage and supply systems for cryogenic propellants and life support fluids also require quantitative data for boiling heat transfer. Additionally, an assessment of the cooling of electronic package or power supply systems associated with various instrumentation and control systems requires a knowledge of boiling heat transfer coefficients and maximum and minimum heat fluxes.

The proposed work will go a long way in developing an understanding of the boiling phenomena in microgravity conditions. This understanding, in turn, will allow for this design and performance prediction of various systems such as those described above.

Progress During FY 1996:

Since the initiation of the project in May, 1996, contacts have been established with researchers doing microgravity boiling heat transfer work in other countries. This includes a visit to the laboratory of Professor Ohta in the Mechanical Engineering Department at the Kyushu University, Japan. Professor Ohta is carrying out low-gravity experiments on pool and flow boiling. This visit was not sponsored by NASA. In addition, ground-based experimental work has been initiated. Silicon wafers with one, two or four cavities have been fabricated. Experimental apparatus to study onset of boiling, bubble growth, and bubble merger processes has been developed. The apparatus consists of a copper block, instrumented with thermocouples and cartridge heaters. The wafer is cemented to one face of the copper block. Liquid pool on the boiling surface of the wafer is formed in a Pyrex channel with a square cross-section. A few preliminary experiments have been successfully conducted with a wafer containing four cavities. Numerical studies conducted so far have included simulation of the bubble shape and velocities induced in the liquid after a bubble detaches from the heater surface. Gravity is an important parameter of the analysis.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 963-25-04

NASA CONTRACT NO.: NAG3-183

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Son, G. and Dhir, V.K., "Non-linear Taylor instability with application to film boiling and melting." Proceedings of the Japan-US Seminar on Two Phase Flow, pp.301-309, July 15-20, 1996.

Presentations

Kugler, S. and Dhir, V.K., "Enhancement of nucleate boiling heat flux on macro/micro structured surfaces cooled by multiple impinging jets." AIChE Symposium Series, vol. 92, pp. 287-293, August 3-6, 1996.

Son, G. and Dhir, V.K., "Numerical simulation of liquid-vapor, liquid-gas, liquid-liquid interfaces subjected to Taylor instability." Presented at the Fluid Engineering Conference of ASME, July -8-12, 1996.

The Melting of Aqueous Foams

PRINCIPAL INVESTIGATOR: Prof. Douglas J. Durian

University of California, Los Angeles

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

To exploit rheological and multiple-light scattering techniques, and ultimately microgravity conditions, in order to quantify and elucidate the unusual elastic character of foams in terms of their underlying microscopic structure and dynamics. Special interest is in determining how this elastic character vanishes, i.e., how the foam melts into a simple viscous liquid as a function of both increasing liquid content and shear strain rate.

Task Description:

The unusual elastic character of foams will be quantified macroscopically by measurement of the shear stress as a function of static shear strain, shear strain rate, and time following a step strain; such data will be analyzed in terms of a yield stress, a static shear modulus, and dynamical time scales. Microscopic information about bubble packing and rearrangement dynamics, from which these macroscopic non-Newtonian properties presumably arise, will be obtained non-invasively by novel multiple-light scattering diagnostics such as diffusing-wave spectroscopy (DWS). Quantitative trends with materials parameters, such as average bubble size, and liquid content, will be sought in order to elucidate the fundamental connection between the microscopic structure and dynamics and the macroscopic rheology.

Task Significance:

The utility and fascination of foams are derived largely from the surprising fact that they have a solid-like elastic character in spite of being mostly gas with a few percent volume fraction of liquid, but can nevertheless flow under shear. The physical origin of such unusual rheology in terms of microscopic structure and dynamics is poorly understood and remains a subject of basic scientific interest to physicists, chemists, and chemical engineers. The proposed research promises important new insight into these issues, and could also have significant consequences for our understanding of flow in other dense randomly-packed systems such as emulsions, colloidal suspensions, slurries, bubbly liquids, and granular materials. Furthermore, all foam applications are empirically based and the proposed research may generate valuable fundamental guidance for the development of materials with more desirable rheology and better stability.

Progress During FY 1996:

During this period we have made progress in designing and building experimental apparatus. In particular we have nearly finished construction of a large shear cell that will permit access for multiple-light scattering diagnostics. Eventually, torque transducers will be added so that the full range of rheology and structure diagnostics will be available in a single apparatus, as intended in the ultimate flight experiments. We have also obtained additional laboratory space that is now being renovated (new fume hood and storage & bench space) prior to the arrival of a commercial rheometer. Furthermore, we have begun exploring how to produce foams with a homogeneous, reproducible bubble size distribution and continuously variable liquid content.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 3

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 963-24-00

NASA CONTRACT NO.: NAG3-184

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Durian, D.J., Gopal, A.D., Vera, M.U., and Langer, S.A. "The melting of aqueous foams." NASA Conference Publication (1996).

II. MSAD Program Tasks — Flight Research

Presentations

Durian, D.J. "The melting of aqueous foams." Third Microgravity Fluid Physics Conference, NASA Lewis Research Center, Cleveland, OH, 1996.

Critical Dynamics of Fluids

PRINCIPAL INVESTIGATOR: Prof. Richard A. Ferrell

University of Maryland

CO-INVESTIGATORS:

Moldover, M.
Wilkinson, R.A.

National Institute of Standards and Technology (NIST)
NASA Lewis Research Center (LeRC)

Task Objective:

This work has three objectives all relating to second-order phase transitions in fluids. Part one seeks to confirm the untested dynamic scaling of the asymptotic limiting acoustic attenuation in simple liquid-vapor systems. The second part seeks to confirm the fast dynamics of adiabatic heat transfer in compressible liquid-vapor critical systems in a space experiment. The third objective is to expand the theory of the specific heat at the lambda transition of liquid ^4He . The theory would allow for comparison with data from a currently planned space experiment, namely CHEX.

Task Description:

The work involved three critical fluid investigations: 1) ground-based definition of an acoustic attenuation in a pure liquid-vapor system space experiment, 2) Analysis of a fast adiabatic thermal/density relaxation space experiment which flew on IML-2 in 1994, and 3) theoretical work on the specific heat near the lambda transition of ^4He . Item 1 involves repeating the Garland & Thoen experiment to establish techniques and demonstrate that adiabatic heat transfer losses are detectable and predictable. That knowledge will be useful in defining a space experiment that will not be hampered by this effect. It is the space experiment that would fulfill the first objective.

Item 2 employed ESA's Critical Point Facility (CPF) with visual and interferometric data. A heat pulsed wire and a 500 Volt charged wire were used to stimulate fast transients and electrostriction. This activity also allowed a reflight of an IML-1 experiment to study slow density relaxation with better geometric and thermal boundary conditions.

Task Significance:

Significance is based on the fundamental character of this work, all of which is driven by experiments only possible in low-gravity. The ^4He work is to bring current theory up to par with experiments in process. The liquid-vapor acoustics work is to test the predictions of dynamic scaling theory, while properly accounting for adiabatic heat transfer loss mechanisms. The experiments on IML-2 also works toward the confirmation of the theory describing adiabatic heat transfer in highly compressible critical fluids.

Progress During FY 1996:

Progress During FY 1996: During the past twelve months, further effort has been devoted to a refinement of the analysis and interpretation of the experiments Fast Adiabatic Equilibrium (AFEQ) and Temperature Equilibration Bis (TEQB) that were flown aboard the space shuttle Columbia in July, 1994. This work was reported by Dr. G. Zimmerli and co-investigator Dr. Wilkinson at the Third Microgravity Fluid Physics Conference at which the P.I. also spoke on some more general aspects of the theory of second order phase transitions.

AFEQ:

An impediment to a direct comparison of the theory of electrostriction with the experimentally observed interferograms is the fact that the optical system of the Critical Point Facility (CPF) does not image the sample cell onto the recording CCD camera, but instead, onto a "virtual" plane. As a consequence, a light ray that has been influenced by the electrostrictive density inhomogeneities in the fluid, and thereby deflected by a small angle, becomes laterally displaced when it impinges on the CCD plane. It is essential to allow for this displacement when interpreting the fringe pattern of the interferograms. A significant obstacle in carrying out such analysis is an uncertainty in regard to some of the parameters of the optical system--in particular, the location of the principal planes of the thick lenses. We have made some progress in eliminating this uncertainty, thereby making possible the preparation of a final and definitive scientific paper on this electrostriction experiment.

TEQB:

The primary goal in TEQB was to measure the rate of heat diffusion at a temperature closer to the critical point than is possible on Earth. The heat flow across the sample cell imposes an initial condition for the temperature relaxation that has an angular dependence that is described by a cosine (or sine) function. An expansion in normal modes is feasible. This has, in fact, been carried out, but it can be argued that the analysis of the relaxation in terms of the "tilt" function that corresponds to the presumed uniform temperature gradient of the initial condition promises greater accuracy. This is because, at every stage of the relaxation, the actual temperature distribution is more closely similar to the "tilt" function than it is to any of the Bessel's functions that describe the individual normal modes. Two alternate methods of implementing the "tilt" function approach have been followed at the University of Maryland and at NASA Lewis Research Center. The Maryland and Lewis results agree above 10mK but exhibit a difference at 10mK. A further troubling discrepancy, also not yet understood, is the failure of the phase map to satisfy the isothermal boundary condition at the cell perimeter. Resolution of these discrepancies will clear the way for a final publication on TEQB.

When the heat flow is turned off in TEQB, the initial condition can be expected to excite not only the "tilt" mentioned above, but also the cylindrically symmetric modes. Alternatively, one expects a flat relaxing temperature distribution with the spatial dependence consisting only of some rounding at the cell perimeter. This is a non-isobaric non-one-dimensional phenomenon for which the theory has not yet been worked out. It is necessary to include adiabatic temperature changes, as described by the now familiar Onuki-Ferrell-Hao differentio-integro-equation. An expansion in eigenfunctions of the Laplace operator yields a solution in terms of a doubly infinite series. This work is still in progress.

Critical Sound Propagation: Measurements have been made by Dr. R Kusner of the acoustic spectrum of a critically filled SF6 resonator at low frequencies ($200\text{Hz} < f < 3000\text{Hz}$). The resonator was an annulus of height 3 mm and circumference 28 cm. The resonator was designed to oscillate at low frequencies in order to probe the effects of surface to volume ratio (or the thermal boundary layer) on the acoustic resonances of a critical fluid. Unfortunately, these data have been beset with spurious resonances, presumably attributable to mechanical oscillations in the metal resonator rather than to pressure waves in the fluid. The unfavorable impedance match between the transducer and the fluid is evidently responsible for this difficulty. On the theoretical side of this project, we have succeeded in developing a crossover correction for experiments that are not carried out entirely in the critical region. A scientific publication on this work is in preparation.

In the low temperature realm, Prof. Bhattacharjee has developed a method for taking into account the effect of boundary conditions on order parameter fluctuations, with a view toward making a prediction for CHeX .

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 12/92 EXPIRATION: 2/96

PROJECT IDENTIFICATION: 963-24-0C-25

NASA CONTRACT NO.: NAG3-139

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Mukhin, S.I., Kyung, B., and Ferrell, R.A., Spin-fluctuation gating in the c-axis non-Drude conductivity of the high T_c cuprates. *Annalen der Physik*, (1996).

Proceedings

Ferrell, R.A., "A brief survey of the equilibrium and transport properties of critical fluids and the degree to which microgravity is required for their experimental investigation." *Proceedings of the Third Microgravity Fluid Physics Conference*, Cleveland OH, NASA Conference Publication 3338, pp. 53-57, June, 1996.

Presentations

Ferrell, R.A., "Modulated order parameter." *Max-Planck-Institut fuer Physik Komplexer Systeme*, Dresden Germany, June, 1996.

Microscale Hydrodynamics Near Moving Contact Lines

PRINCIPAL INVESTIGATOR: Prof. Stephen Garoff

Carnegie Mellon University

CO-INVESTIGATORS:

Weislogel, M.

NASA Lewis Research Center (LeRC)

Task Objective:

The study will characterize the unique hydrodynamics occurring in a microscopic region near moving contact lines and controlling macroscopic spreading of fluids on solid surfaces.

Task Description:

Using very accurate optical imaging techniques and particle image velocimetry, we characterize the shape of the fluid/fluid interface and the flow fields in a microscopic region near moving contact lines. From these images, we test models of the hydrodynamics in regions near the contact line where viscous forces dominate the fluid flow and in regions even closer to the contact line where a unique hydrodynamic regime must govern the fluid motion. By making systematic changes in the materials system under examination, we seek the physical origins of these unique hydrodynamics. Low gravity studies are essential to this program, removing the masking influence of the macroscopic fluid flow from the regions of interest.

Task Significance:

The task significance is to 1) Establish the correct method for measuring dynamic contact angle boundary condition, 2) Provide a proper basis for predictive models of spreading, 3) Test models of the hydrodynamics near, but not at, moving contact lines where viscous forces are dominant, and 4) Identify the molecular-scale mechanisms governing the unique hydrodynamic regimes at moving contact lines.

Progress During FY 1996:

We have continued our study of asymptotic spreading models through quantitative analysis of the flow field near moving contact lines. As a polymer liquid spreads on a surface, we make simultaneous measurements of the interface shape and flow field in the first few hundred microns from the contact line. The no-slip boundary condition at the solid-liquid interface holds at least as close as 100 microns from the contact line at $Ca=0.43$. The "modulated wedge" solution, central to the asymptotic models under investigation, holds for $Ca < 0.10$ but breaks down for higher Ca . This breakdown is caused by violation of the small curvature assumption of the model. These results are consistent with our results on the breakdown of the interface shape models for the same Ca . Even when the analytic models of spreading break down, numerical calculations of the fluid spreading can be performed in the intermediate and outer regions where the Navier-Stokes equation and the classical hydrodynamic boundary conditions hold. Our simultaneous measurements of the interface shape and velocity fields in the geometry free region form needed boundary conditions for such numerical calculations.

We have explored the role of thin films in moving contact lines. Spontaneous precursing films of 100cST polydimethylsiloxane form on clean pyrex. However, they form slowly and do not exist even for contact line speeds as slow as 5 microns/sec. Thus, they are not the inner scale mechanisms dominating over the Ca ranges where viscous forces are playing important roles in spreading. We have begun a study of fluids advancing over pre-existing thick (on the order of microns) films. At lower Ca , our first measurements agree with a model which asymptotically matches an inner solution based on the lubrication approximation to a static outer solution with zero contact angle.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 4/96 EXPIRATION: 4/00

PROJECT IDENTIFICATION: 963-25-OH

NASA CONTRACT No.: NCC3-465

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Chen, Q., Rame, E., and Garoff, S., Experimental studies on the parametrization of liquid spreading and dynamic contact angles. *Colloids and Surfaces*, (1996).

Chen, Q., Rame, E., and Garoff, S., The velocity field near moving contact lines. *J. of Fluid Mech.*, (1996).

Rame, E., and Garoff, S., Microscopic and macroscopic dynamic interface shapes and the interpretation of dynamic contact angles. *J. Colloid Interface Sci.*, vol. 177, 234 (1996).

Presentations

Rame, E., "Physics of liquid spreading." Pennsylvania State U., March, 1996.

Rame, E., "Hydrodynamics near moving contact lines." Carnegie Mellon Polymer Symposium, May, 1996.

Rame, E., "Hydrodynamics of moving contact lines." Institute for paper science and technology, May, 1996.

Rame, E., "Microscale hydrodynamics near moving contact lines." Third Fluids Microgravity Conference, NASA LeRC, Cleveland, OH, June, 1996.

Geophysical Fluid Flow Cell

PRINCIPAL INVESTIGATOR: Dr. John E. Hart

University of Colorado, Boulder

CO-INVESTIGATORS:

Leslie, F.
Miller, T.
Ohlsen, D.

NASA Marshall Space Flight Center (MSFC)
NASA Marshall Space Flight Center (MSFC)
University of Colorado, Boulder

Task Objective:

The Geophysical Fluid Flow Cell experiment (GFFC) takes advantage of the unique environment of the microgravity laboratory, which permits forces that would otherwise be swamped by normal terrestrial gravity to become dominant. The GFFC uses electrostatic forces to warp gravity into a radial vector field, centrally directed towards the center of the cell. This allows us to perform visualizations of thermal convection in a spherical shell of liquid subject to imposed differential heating and basic rotation, where the active buoyancy forces are radially directed, as in planetary atmospheres and stars. The objective of the experiments is to categorize the types of convective patterns that can occur in highly nonlinear and turbulent flows with varying amounts of basic rotation and thermal stress.

Task Description:

1. Preparation of the GFFC instrument, including its new real-time video acquisition hardware. Testing and calibration of the hardware. Construction of scenarios to be programmed for operation during the USML-2 mission.
2. The film images and video images will be transferred to video laser disc, and programs permitting rapid access to the data will be written. These allow comparisons of images from different runs, as well as the construction of easy animation from the experiment, showing time histories of the convection.
3. Theoretical and computational models typically involve assumptions that will be checked using the data from the Spacelab flights.

Task Significance:

The spherical configuration and radial gravity of the Geophysical Fluid Flow Cell is significant because large-scale motions of the atmospheres of planets and stars are constrained by the inherent spherical geometry of these bodies. Furthermore, the flows on them are constrained by rotation, under the action of the same Coriolis forces that shape Earth's weather, and by buoyancy forces which result in hot fluid rising in a radial direction. It is impossible to study such motions in the terrestrial laboratory because gravity is uniformly directed. The GFFC experiments will provide basic laboratory data that can be applied to problems of cloud patterns on the giant planets, differential rotation on the Sun, and motions in Earth's core, mantle and atmosphere.

Progress During FY 1996:

1. Preparation and testing of flight hardware was completed.
2. The flight of GFFC on USML-2 was completed in November 1995.
3. Data films and tapes were received in May 1996 and transferred to video disk.
4. Initial analysis of operation of the experiment was carried out, and preliminary comparisons with computational simulations were addressed.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	2	MS Degrees:	1
PhD Students:	0	PhD Degrees:	0

TASK INITIATION: 12/88 EXPIRATION: 10/96

PROJECT IDENTIFICATION: 963-25-15

NASA CONTRACT No.: NAS8-319

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Hart, J.E., and Kittelman, S. Instabilities of the sidewall boundary layer in a differentially driven rotating cylinder. Physics of Fluids, vol. 8, 692-696 (1996).

Hart, J.E., and Mundt, M.D. Instability of oscillatory Stokes-Stewartson layers. J. Fluid Mech., vol. 311, 119-140 (1996).

Growth and Morphology of Phase Separating Supercritical Fluids

PRINCIPAL INVESTIGATOR: Dr. John Hegseth

University of New Orleans

CO-INVESTIGATORS:

Beysens, D.

Garrabos, Y.

Perrot, F.

Nikolayev, V.

French Atomic Energy Commission

University of Bordeaux, France

French Atomic Energy Commission

French Atomic Energy Commission

Task Objective:

The objective of this work is to study the relations between off-critical density, domain morphology, and the scaling power of the time growth of domains during phase separation of near-critical pure fluids in microgravity.

Task Description:

Previous work has shown that for critical density samples late stage domain growth is linear in time with the domains having an interconnected morphology. Sufficiently off-critical density samples show late stage domain growth that has a cube-root of time growth law and disconnected domain morphology. The investigator group has proposed a simple theory to explain the two growth regimes.

The plan is to vary the off-critical density of samples to map out the crossover between the two growth laws and morphologies. The results will then be compared to the existing model of the investigators.

Existing space experiment apparatus will be used for the experiments. Careful attention will be paid to density gradients induced by temperature quenches, which in the past limited the precision of results.

Task Significance:

This work seeks to improve the fundamental understanding of phase separations which have long been common in the science and technology.

Progress During FY 1996:

We are in the process of testing a variable volume critical fluid cell. We are also examining fluid dynamical instabilities that have occurred in similar microgravity experiments. Another MIR mission has just finished that used the ALICE II instrument. The results of this experiment will be relevant to the proposed experiment. These results will be available in several months.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 963-25-OH

NASA CONTRACT NO.: NAG3-190

RESPONSIBLE CENTER: LeRC

An Experimental Study of Richtmyer-Meshkov Instability in Low Gravity

PRINCIPAL INVESTIGATOR: Dr. Jeffrey W. Jacobs

University of Arizona

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

To carry out ground-based experiments to study the nonlinear development and transition to turbulence of Richtmyer-Meshkov instability. To develop a flight experiment based on the ground-based apparatus in order to utilize the low gravity environment of space for the creation of an experiment with virtually unlimited duration.

Task Description:

Richtmyer-Meshkov instability occurs when a planar interface separating two fluids of different density is impulsively accelerated in the direction of its normal. The focus of this research project is to observe and quantify the nonlinear development of this instability from a simple well characterized initial state into a turbulent flow, and to determine whether a self-preserving final turbulent state is achieved. The experiments utilize a novel experimental apparatus which circumvents many of the experimental difficulties that have previously limited the study of Richtmyer-Meshkov instability. In this system, the instability is generated by bouncing a thin rectangular tank containing two liquids off of a fixed spring. Because the run time in these experiments is limited, and the length of time necessary to characterize the final turbulent state is unknown, experiments will be carried out in a series of steps in which progressively longer run times can be achieved. First, planar laser induced fluorescence imaging will be implemented in a presently existing apparatus to improve visualization capabilities and provide measurements of mixing. Next, a new apparatus will be constructed, whereby longer run times will be achieved. In addition, a space-based experiment, similar in principle to the current ground-based experiment, will be designed in order to obtain further increases in run time.

Task Significance:

Richtmyer-Meshkov instability is one of the most fundamental of fluid instabilities and is of importance in fields ranging from astrophysics to materials processing. For example, Richtmyer-Meshkov instability is of critical importance to inertial confinement fusion. The degree of compression capable in laser fusion experiments is ultimately limited by Richtmyer-Meshkov instability and another similar instability called Rayleigh-Taylor instability. Thus, these instabilities represent the single most significant barrier to attaining positive-net-yield fusion reactions in laser fusion facilities. Richtmyer-Meshkov instability is also of importance to high speed combustion applications, where, for example, it can greatly enhance mixing and thus significantly alter the burning rate. Knowledge gained from this study should aid in the design of laser fusion targets and supersonic combustors.

Progress During FY 1996:

Work has begun on the implementation of planar laser induced fluorescence in the existing experimental apparatus. Preliminary experimental results utilizing this system are very promising and provide a much clearer picture of the instability. Work has also begun on an improved initial condition generation system which will enable the generation of a much wider variety of initial surface shapes.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/00
PROJECT IDENTIFICATION: 963-25-OH
NASA CONTRACT NO.: NAG3-186
RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Jacobs, J.W. and Niederhaus, C.E., "An experimental study of Richtmyer-Meshkov instability." NASA 3rd Fluids Physics Conference, NASA Lewis Research Center, June 13-15, 1996.

Microgravity Segregation in Binary Mixtures of Inelastic Spheres Driven by Velocity Fluctuation Gradients

PRINCIPAL INVESTIGATOR: Prof. James T. Jenkins

Cornell University

CO-INVESTIGATORS:

Louge, M.

Cornell University

Task Objective:

The objective of this work is to investigate rapid granular flows of dry materials in reduced gravity. In rapid flows, the particles interact through collisions, and the energy of the particle velocity fluctuations plays an important role in the physics. This research will focus on the separation of grains by properties (e.g. size) that is driven by spatial gradients in the fluctuation energy of the grains.

Task Description:

Conventional shear cells used to investigate rapid granular flows consist of a circular path in which the grains are allowed to move, thus creating large centrifugal forces that promote condensation of the granular mass near the outer wall of the cell. In microgravity environments, it is crucial to avoid centrifugal forces. Consequently, in this effort, a novel design of a microgravity shear cell will be employed. This shear cell will be composed of two linear test sections. The cell consists of a stationary shell and a moving belt. The belt is made up of chain links for strength and flexibility. It is engaged by two large rollers at each end of the cell. Steel spheres are attached to the belt to provide the surface texture of the moving boundary. The spacing of these spheres is adjusted to balance the production and dissipation of granular temperature at the boundary. The stationary wall of the top test section is roughened in a similar manner, but the spacing is such that the boundary provides fluctuation energy to the flow. Conversely, the stationary wall of the bottom test section is engineered to dissipate that energy. The intent of this work is to compare the segregation behavior of the two sections with different energetics. To accomplish this, the cell will be filled with a mixture of two types of spherical grains. The grains will be driven to interact with the two types of boundaries on either side of the cell. The resulting separation will be observed visually.

Earth-bound cells use large shear rates to increase the particle pressure and reduce the influence of gravity. However, the intense shearing produces considerable damage to the test spheres. This creates microscopic dust that provides artificial lubrication to the collisions. For ductile materials, another difficulty is that the coefficient of restitution decreases as the impact velocity increases. The resulting corruption of data is unpredictable. Because the peak contact force is roughly proportional to the impact velocity, serious damage to the test spheres and degradation of the restitution can be avoided by limiting the shear rate. The microgravity environment permits us to do this.

In this work, theoretical analysis and numerical simulations will be carried out of the collisional momentum and energy transferred to the flow from a bumpy, frictional shear cell. The results of these analyses will be used in the fabrication of a prototype shear cell. Using this prototype, experiments to test the operation of the cell will be carried out aboard the microgravity aircraft. Video will be used to observe the possibly incomplete segregation. Visually and using existing instruments, the impact parameters will be measured for binary collisions of test spheres, and for collisions of these with bumpy boundaries. The results obtained from these experiments will be used in the design of the flight shear cell.

Task Significance:

The size segregation of flowing or shaken grains is a commonly observed phenomenon in industrial processes and in nature. In many industrial processes a homogeneous aggregate is desired; in these size segregation is undesirable. However, in the mining industry, segregation by size is exploited in some crushing operations. When observing natural grain deposits, grain segregation provides an indication of whether an aggregate of grains was deposited dry (larger grains above) or under water (larger grains below).

In systems that do not involve much agitation of the grains, several mechanisms that involve gravity have been identified as leading to such segregation. In highly agitated flows there is a mechanism independent of gravity that is available to drive separation. This is associated with spatial gradients in the energy of the velocity fluctuations

II. MSAD Program Tasks — Flight Research

of the grains. Collisional interaction between and among different species of grains require that, in general, spatial gradients of concentration exist to balance spatial gradients of the particle fluctuation energy. In rapidly sheared or vibrated systems, gravity also influences mixtures of different size grains. Here, buoyant forces act to separate grains that differ in size and the local volume that they displace.

In reduced gravity, buoyant convection is suppressed and attention can be focused on the simpler balance between gradients in concentration and the gradients in fluctuation energy. Reduced gravity also eliminates the possibility that a rapid flow will condense into a slower, denser flow dominated by enduring contacts rather than by collisions. Also, microgravity makes the visual observations possible by permitting one to employ moderate rates of shear. On Earth, the effects of gravity can be minimized by shearing so rapidly that the particle pressure overwhelms gravity. However, in this event, separation takes place too rapidly for visual observation. Also, buoyancy and/or condensation associated with the centripetal acceleration must be taken into account, and the particles can be severely damaged.

Progress During FY 1996:

Theory:

Characterized bumpy boundary by relating separation and diameter ratio to average angle penetration.

Determined profiles of fluctuation velocity and mean velocity for the shearing of dense systems between two different bumpy frictionless boundaries when gravity is negligible.

Completed corrected determination of the energy flux at a flat frictional wall.

Determined top and bottom bumpy frictionless boundaries that provide the greatest gradient in fluctuation energy.

Engaged researchers at Rennes in an experimental study of segregation driven by gradients of fluctuation energy in 2D shearing flows of a binary mixture of disks on their air table.

Engaged Kevin Craig at RPI in an experimental study of segregation driven by gradients of fluctuation energy in 3D shearing flows of a binary mixture of spheres in his shear cell.

Simulation:

The corresponding computer code is nearly complete. Its capabilities are:

- complete simulation of the entire shear cell with spheres of arbitrary diameter and mass;
- boundary preparation with spheres packed on hexagonal or square patterns or with cylindrical bumps;
- measurement of volume fraction, mean velocity and granular temperature of two species;
- generation of files for virtual reality video production;
- independent movement of inner and outer boundaries;
- investigation of the fully developed region through periodic boundary conditions.

Design:

Completed a preliminary paper design of the cell mockup. It uses a chain drive to move the inner boundary. The PI contemplates attaching cylindrical bumps to plates riveted to the chain links. An advantage of this configuration is firmness of the underlying boundary upon granular impact.

Evaluating and modifying software packages for video image recognition and analysis to provide the location and velocity of particle centers with sufficient accuracy to measure spatial gradients of concentration and fluctuation velocity.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 0

TASK INITIATION: 4/96 EXPIRATION: 4/00
PROJECT IDENTIFICATION: 963-25-OH
NASA CONTRACT No.: NCC3-468
RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Jenkins, J.T. and Hanes, D.M. A sheared sheet of colliding grains driven from above by a turbulent flow. *J. of Fluid Mechanics*, (in press).

Jenkins, J.T. and Louge, M.Y. On the flux of fluctuation energy through a flat, frictional wall bounding rapid flows of inelastic frictional spheres. *Physics of Fluids*, (1996).

Proceedings

Jenkins, J.T. and Louge, M.Y., "Microgravity Segregation in Binary Mixtures of Inelastic Spheres Driven by Velocity Fluctuation Gradients." *Proceedings of the Third Microgravity Fluid Physics Conference, NASA, 1996.*

Presentations

Jenkins, J.T., "Inelastic behavior of random arrays of identical spheres." *UTAM Symposium on the Mechanics of Granular and Porous Materials*. (N.A. Fleck and A. Cocks, Eds.) Kulwer, Sandia Labs, 1996.

Bubble Dynamics on a Heated Surface

PRINCIPAL INVESTIGATOR: Dr. Mohammad Kassemi

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

Rashidnia, N.
Mercer, C.R.

NYMA, Inc.
NASA Lewis Research Center (LeRC)

Task Objective:

The objective of this combined experimental/numerical work is to investigate the transient evolution of fluid flow and temperature fields in the vicinity of a bubble attached to a heated solid surface. The research effort is focused on clarifying the interaction between thermo-capillary and natural convective flows in the vicinity of the bubble and identify numerically the parametric range for which unsteady periodic oscillations occurs on earth and in the low-gravity environment. It is hoped that the experience gained during this investigation will aid in designing and proposing the right space experiment.

Task Description:

The oscillatory thermo-capillary phenomenon is not only of fundamental importance in understanding the behavior of fluid flow in space but it also has practical significance in terrestrial applications. For example, in crystal growth, the oscillatory temperature and flow fields created by unavoidable bubbles next to the solid-liquid interface may seriously affect the quality of the emerging crystal and in nucleate boiling the presence of bubbles on the solid surface may increase the heat transfer rates considerably. The results of this investigation will enhance our understanding of the role of capillary forces in fluid management, boiling processes, and materials processing for both space and ground-based applications.

Task Significance:

The ground-based research activity encompasses the development of a transient numerical model, and improvement of the existing experimental set-up, procedures, and diagnostic techniques for studying the time evolution of thermocapillary and natural convective flows in the vicinity of a gas bubble placed on a heated surface. The fidelity of the model is assessed by comparing numerical predictions to experimental measurements. Hand-in-hand numerical simulations and carefully controlled experiments will be used to identify the parametric range for initiation of temperature and flow field oscillations. The verified numerical model will be used to predict the time evolution of bubble shape, temperature field, and flow structure in the low-g environment. Parametric studies will be conducted to see if the oscillatory phenomenon which is observed in ground-based experiments is also present in the microgravity space environment and to clarify the origin and nature of the oscillations.

Progress During FY 1996:

Both theoretical and experimental accomplishments were made in FY96. The existing test cell setup was modified to expand and fine-tune the parametric range of Ma and Ra numbers. This is needed for studying the initiation of the various oscillatory modes and is accomplished through improved control of the imposed temperature gradient and bubble size.

The diagnostic techniques were also improved by adopting the Wollaston Prism Interferometry (WPI) technique and developing an Abel transformation computer code to extract temperature data from the interferometry results.

A transient finite element model was developed and used to study the time evolution of thermocapillary convection and temperature field around the bubble. Preliminary transient simulations below the critical Ma number indicate that as soon as the bubble is subjected to the imposed axial temperature gradient, a strong thermocapillary flow is initiated. Gradually, a recirculating vortex develops with its center positioned near the bubble and the hot plate. As the flow intensifies, the center of the vortex tends to move downwards. In 1-g, the upward push by the buoyancy force restricts this tendency and maintains the center of the vortex in the vicinity of the bubble. As the flow stabilizes, the shear force exerted by it on the fluid below the bubble induces secondary and tertiary recirculating cells. Low-G transient simulations exhibit the same initial behavior. However, due to the absence of the buoyancy

force in low gravity, as the flow intensifies, the thermocapillary vortex grows and expands until a single recirculating cell occupies the whole domain.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/96 **EXPIRATION:** 10/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NCC3-490

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Kassemi, M., Rashidnia, N., and Mercer, C., "Low-G and 1-G velocity and temperature fields in the vicinity of a bubble on a heated surface." The Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 1996.

Interfacial Phenomena in Multilayered Fluid Systems

PRINCIPAL INVESTIGATOR: Prof. Jean N. Koster

University of Colorado, Boulder

CO-INVESTIGATORS:

Biringen, S.

University of Colorado, Boulder

Task Objective:

The main objective of the grant was to systematically develop a program of research to study various aspects of (mainly) immiscible multilayered fluid systems which would eventually lead to the design of a Shuttle flight experiment. These studies were confined to the study of single, double, and triple liquid layer systems. These systems had multiple liquid layers with parallel interfaces undergoing either natural convection, Rayleigh-Bénard convection, and/or thermocapillary convection effects. These various types of convection were imposed by temperature gradients either parallel to or perpendicular to the fluid interfaces. Of particular interest were the mechanical and thermal coupling effects across the interfaces as well as the interaction of the flow patterns between adjacent liquid layers. In addition, it was also of interest to investigate the possible suppression of convective flow in one of the fluid layers.

Task Description:

This grant effort was begun in November 1989 and was completed in December 1995. As mentioned above, the general approach was to conduct a systematic program of ground-based (normal-gravity) testing leading to the development of and the execution of a Shuttle based-flight experiment. Flight hardware was built (by ESA/ESTEC) and flew on the Bubble Drop Particle Unit (BDPU) on the Second International Microgravity Laboratory (IML-2) in June of 1994. Theoretical models for the combined buoyant and thermocapillary convection phenomena were developed during the course of this grant. The theories and numerical models developed, not only, verified the one-g data, but were also used to predict anticipated results of the flight experiment. Unfortunately the experiment was not successful. All of the data from this effort is, therefore, one-g data. From October 1995 to December 1995 when this effort ended, the main efforts were to continue to perform and document the normal gravity multilayer experiments in the lab that continued after the unsuccessful IML-2 experiment.

Task Significance:

The results significantly advance our knowledge in the areas of surface-tension-driven convection, natural convection, and Rayleigh-Bénard convection (and combinations of these) as applied to multilayered fluid systems. Of particular scientific interest are the coupling mechanisms between adjacent fluid layers and subsequently knowledge of how to control fluid flows in interior liquid layers. These scientific results find direct applications in fields related to encapsulated float zone processing. Float zone processes are commercial techniques which are used to grow crystals. It is thought that if such processes can be done in space that these processes will result in large crystals with relatively few imperfections.

Progress During FY 1996:

As was mentioned above, the IML-2 flight experiment attempted in June 1994 was not successful. ESA/ESTEC, however, decided to re-fly a modified/improved version of Prof. Koster's IML-2 test container on the LMS mission under the auspices of a European investigator, J. C. Legros of Belgium. Prof. Legros had a very similar three-liquid-layer experiment on IML-2 also. He therefore was very familiar with the physics behind the Koster experiment. The experiment flew very successfully on the LMS mission in June 1996. The data is currently being analyzed by Prof. Legros' team at ULB; whose efforts are not the direct result of any NASA funding.

The NASA funded grant activities have concluded as of December 1995 and were a continuation of the ground-based efforts after the IML-2 mission. The multifaceted ground-based program of Prof. Koster continued to study the many aspects of multilayered flows. The specific areas of study, as previously reported included: natural convection in single, double, and triple layers; Rayleigh-Bénard convection (instability studies) in double layers with one gas interface; and combined natural and Rayleigh-Bénard convection in double layers. For the natural convection cases thermocapillary effects had varying degrees of influence depending upon the physical parameters. In addition, some of the above cases were done not only with immiscible fluids but with partially miscible fluids as well. Fluids

exhibiting density inversions were also studied. Two significant findings of this effort were the defining of conditions in which the flows in the middle of a three layer system were suppressed; and also conditions were found in which multiple roll cells existed in interior liquid layers. The research results have been disseminated through 24 publications in referred journals and 15 conference presentations.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	3
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 11/89 **EXPIRATION:** 12/95**PROJECT IDENTIFICATION:** 963-24-00-05**NASA CONTRACT NO.:** NAG3-109**RESPONSIBLE CENTER:** LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Campbell, T. and Koster, J.N. Modeling on convection in Gallium encapsulated by silicone oils. *Acta Astronautica*, vol. 35, 805-812 (1995).

Koster, J.N. and Nguyen, K. Steady natural convection in a double layer of immiscible liquids with density inversion. *Int. J. Heat Mass Transfer*, vol. 39, 467-478 (1996).

Prakash, A. and Koster, J.N. Steady Rayleigh-Benard convection in a two-layer system of immiscible liquids. *J. Heat Transfer*, vol. 118, no. 2, 366-373 (1996).

Prakash, A. and Koster, J.N. Steady natural convection in a GaAs melt encapsulated by molten B_2O_3 . *J. Material Synthesis and Processing*, vol. 4, no. 1, 43-50 (1996).

Magnetorheological Fluids: Rheology and Nonequilibrium Pattern Formation

PRINCIPAL INVESTIGATOR: Prof. Jing Liu

California State University, Long Beach

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This research investigates experimentally the influence of gravity in the formation of the equilibrium structure of magnetorheological fluids.

Task Description:

Magnetorheological (MR) fluids are colloidal suspensions whose rheological properties can be varied through the application of an external magnetic field. The key to this modification is the structure induced in the particles of the suspension. This work focuses on a better understanding of both equilibrium and nonequilibrium structures as well as their influence on rheology and the influence of gravity on their formation. Our previous measurements are the basis for this effort. We will start our research by continuing our measurements on the dynamics in dilute samples and extending these to more concentrated samples. At the same time we begin our rheology measurements by comparing the effect of equilibrium structures to nonequilibrium structures. The basic experimental techniques for this work will be static laser light scattering, dynamic light scattering, optical microscopic imaging, and rheology.

Task Significance:

This research will help us to understand the basic physics of the structure formation in this so called "smart" material under the application of an external field. It will additionally provide guidelines for applications of MR fluids as technologically important materials. For example, this material can be used in automobiles as shock absorbers, clutch controls, robotic joint controls, etc., due to the viscosity change controlled by the field. In order to fully exploit the possibilities of MR fluids and to build more efficient devices, a better understanding is essential.

Progress During FY 1996:

This project which started June 96 is a direct continuation of the work done under NASA grant (NAG3-1634). The FY95 task progress report summarizes our previous work and provides the basis for the current project. In June and July we performed more dynamic light scattering measurements on dilute samples. As a check that the observed oscillations in the correlation function are really caused by the chains i.e. the magnetic field, we measured the scattering angle dependence of the correlation function for different particle sizes and concentrations with no magnetic field applied. No oscillations were observed. Therefore, we conclude that the oscillations observed earlier in dynamic light scattering are due to chain fluctuations.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 2
PhD Students: 1

TASK INITIATION: 6/96 EXPIRATION: 6/97

PROJECT IDENTIFICATION: 963-25-OH

NASA CONTRACT NO.: NAG3-183

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Liu, J., "Chain dynamics in a dilute magnetorheological fluid." Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, 6/13-6/15, 1996.

Presentations

Liu, J., and Hagenbuechle, M., "Chain dynamics in a dilute magnetorheological fluid." Proceedings at Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June, 13-15, 1996.

Extensional Rheology Experiment

PRINCIPAL INVESTIGATOR: Prof. Gareth H. McKinley

Harvard University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this work is to determine the transient extensional viscosity in uniaxial stretching flow for dilute polymer solutions and subsequent relaxation behavior after extensional deformation. To generate a simple homogeneous shear free flow in the material while measuring the stress response of the material during this constant strain rate deformation. To measure the transient birefringence during deformation and relaxation.

Task Description:

This effort will require an initial ground-based experimental design, and ultimate payload implementation on a sounding rocket, of a novel experimental apparatus to measure accurately the rheological response of non-Newtonian fluids under shear-free conditions that are characteristic of those experienced in the containerless processing of materials.

The proposed instrument generates a homogeneous, uniaxial fluid filament through stretching of the test sample. The spatial uniformity, experienced by the fluid, is verified by digital particle image velocimetry. Direct measurements of the tensile force exerted by the material and the column diameter then allow calculation of the extensional viscosity of the fluid. Internal stresses of the polymer chains will be estimated using birefringence. The envisioned apparatus will result in a flexible and adaptable scientific instrument that can accommodate various classes of non-Newtonian liquids and will be suitable for multiple flight capabilities or long term multi-user operation aboard a permanent orbital platform.

Task Significance:

The extensional viscosity is a fundamental physical property of all non-Newtonian materials, and cannot be determined from simple viscometric shear flow experiments. Constitutive equations for viscoelastic fluids such as dilute polymer solutions predict large changes in the extensional viscosity as the elongation rate is increased; however, the validity of these theories cannot be confirmed due to the lack of experimental data obtained in extensional flows. To date, quantitative rheological measurements in shear-free flows have only been possible for highly elastic or "stiff" materials such as polymer melts which can easily be elongated without sagging under a gravitational body force. By performing similar experiments in an extended microgravity environment it will be possible for the first time to obtain accurate measurements of the extensional viscosity for more 'mobile' fluids such as polymer solutions, suspensions and liquid crystalline materials. This rheological data will allow designers of both space- and ground-based material processes to use improved constitutive models in numerical simulations of complex two- and three-dimensional fluid flows.

In a simple stretching flow, fluids such as water or syrup exhibit a resistance to stretching that is exactly three times the value of their Newtonian viscosity. This resistance is usually termed the "extensional viscosity of the material." However, for fluids containing long macromolecules (e.g., synthetic polymers, liquid crystals, or DNA) it is predicted that the extensional viscosity can be anywhere from 100 to 10000 times greater than the viscosity of the fluid. In the near future, NASA plans to develop "containerless processing" operations under microgravity and a detailed understanding of extensional properties in fluids will be absolutely critical -- since, in the absence of container walls, the only way to mix, pour, and shape fluids will be through pure stretching motions. Knowledge of such nonlinear material functions is fundamental to the development and verification of relatively cheap ground-based computational modeling techniques which can be used effectively in the "a priori" design of advanced microgravity material processes thereby alleviating the need for costly in-flight pilot experiments. Finally, in addition to their significance in many industrial processes such as fiber-spinning and film coating operations, stretching flows of non-Newtonian fluids are of fundamental scientific importance to a number of complex fluid dynamics phenomena, including the stability and breakup of jets, enhanced oil recovery and turbulent drag reduction for advanced aircraft, boats, and submarines.

Progress During FY 1996:

The Requirements Definition Review (RDR) was completed on July 17, 1996. The status of the following tasks was presented at the RDR: The third draft of the Science Requirements Document was finished. The birefringence system has been built, assembled and preliminary testing completed. Optical measurements of the fluid filament radius and seeded fluid particle velocities were successfully demonstrated. DPIV software developed at Harvard University was used for the velocity and velocity gradient computations. A laboratory electronic force balance has been identified and tested. A 4:1 reducing diameter device (RDD) was successfully developed. A linear drive unit was designed, built, and used to conduct numerous axial stretching tests of a Boger fluid column with the functioning RDD and electronic force balance attached. The extensional viscosity, and trouton ratio was computed from the resulting force and radius measurements. Inertial motion laboratory tests were conducted using the linear drive mechanism in the neutral density fluid. The secondary flow generated did disturb the polymer filament in these tests. This suggests the desired extensional viscosity data would be in question if the experiment were conducted on earth in this manner. After careful analysis the selected fluid is a dilute, monodisperse polystyrene solution. Surface tension tests were conducted to determine the correlation between the dynamic surface tension and the extensional rheology experiment. The static surface tension was also measured.

The Extensional Rheology Experiment will be flown on a sounding rocket. The experiment will be divided into two sections: the experiment package (EP) and the avionics package (AP). The payload will operate autonomously in flight. Two test points will be performed on each flight. Since the PI has requested 10 test points, five sounding rockets are required.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 12/95 EXPIRATION: 11/00
PROJECT IDENTIFICATION: 963-25-0A-36
NASA CONTRACT NO.: NAG3-179
RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Spiegelberg, S.H., Ables, D.C. and McKinley, G.H., The role of end-effects on measurements of extensional viscosity in viscoelastic polymer solutions with a filament stretching rheometer. *J. Non-Newtonian Fluid Mech.*, vol. 64, 229-267 (1996).

Spiegelberg, S.H. and McKinley, G.H., Stress relaxation and elastic decohesion of viscoelastic polymer solutions in extensional flow. *J. Non-Newtonian Fluid Mech.*, (1996).

Presentations

Spiegelberg, S.H. and McKinley, G.H., "Elastic and viscous contributions to stress in extensional rheometry of viscous polymer solutions." *Proc. XIIth Int. Congr. on Rheology, Quebec City, Canada*, vol.1, 211, 1996.

Spiegelberg, S.H., and McKinley, G.H., "The extensional rheology of non-newtonian materials." *Proc. from the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH*, 1996.

Study of Two Phase Gas-Liquid Flow Behavior at Reduced Gravity Conditions

PRINCIPAL INVESTIGATOR: Dr. John McQuillen

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

Fabre, J.
Colin, C.

Institut De Mecanique Des Fluides, Toulouse ,France
Institut De Mecanique Des Fluides, Toulouse, France

Task Objective:

The objective of this study is to examine the behavior of gas-liquid flows in reduced gravity, specifically for bubble and slug flow and flow through sudden changes in test section diameter.

Task Description:

Reduced-gravity experiments will be conducted on NASA and CNES aircraft to measure the previously listed two-phase flow parameters for a range of tube diameters, gas and liquid flow rates, and fluid properties. There are two thrusts; a ground-based reduced gravity effort and a space-flight experiment as part of the Two-phase Extended Evaluation in Microgravity (TEEM) experiment.

For the ground-based efforts, some experiments will utilize air as the gas phase and aqueous solutions, water, water-glycerin mixtures, and water-zonyl mixtures, for the liquid phase. Additional experiments utilizing an aircraft experiment that is being planned will utilize Freon-134a vapor and liquid. A theoretical modeling effort was integrated with the experimental efforts.

Task Significance:

The purpose of this study is to achieve a better understanding-better predictability-of two-phase (gas-liquid) flow in pipes to assist in the design of space-based power and thermal management systems and of the terrestrial-based nuclear power plants and oil and natural gas pipelines.

Progress During FY 1996:

A set of experiments for air-water flow through two sizes of contractions were conducted in April. The flow regime was visualized and the film thickness and void fraction measurements both upstream and downstream of the contraction were obtained. A dryout that appeared to be pinned at the edge of the contraction was observed for limited flow conditions.

The test section for the TEEM experiment is also being defined to include liquid film thickness and void fraction sensors based on the capacitance technique. Hot film anemometers are being developed for the measurement of wall shear stress.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 3/96 EXPIRATION: 3/00
PROJECT IDENTIFICATION: 963-25-OH
RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

McQuillen, J., Observations of gas-liquid flows through contractions in microgravity. NASA Conference Publication, 3338, pp. 95-102 (1996).

Pool Boiling Experiment

PRINCIPAL INVESTIGATOR: Prof. Herman Merte, Jr.

University of Michigan

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The program described here seeks to improve the understanding of the fundamental mechanisms that constitute nucleate pool boiling. The vehicle for accomplishing this is an investigation, including experiments to be conducted in microgravity and coupled with appropriate analyses, of the heat transfer and vapor bubble dynamics associated with nucleation, bubble growth or collapse, and subsequent motion. Certain effects that can be neglected at normal Earth gravity, such as surface tension and vapor momentum, can become quite significant in microgravity. Momentum imparted to the liquid by the vapor bubble during growth tends to draw the vapor bubble away from the surface, depending on the rate of growth, which in turn is governed by the temperature distribution in the liquid. Thermophoretic forces, arising from the variation of the liquid-vapor surface tension with temperature, on the other hand, tend to move the vapor bubble toward the region of higher temperature. The bubble motion will be governed by which of these two effects prevail.

The elements of nucleate boiling, for which research conducted under microgravity would advance the basic understanding, are:

1. Nucleation or onset of boiling. Indications are that both heater surface temperature and temperature distribution in the liquid are necessary to describe nucleation.
2. The dynamic growth of a vapor bubble in the vicinity of the heater surface. This includes the shape as well as motion of the liquid-vapor interface as growth is taking place. These are influenced by the liquid temperature distribution at the initiation of growth.
3. The subsequent behavior of the vapor bubble. This includes the motion, whether departure takes place or not, and the associated heat transfer.

Task Description:

In the proposed experiment, a pool of liquid—initially at a precisely defined pressure and temperature—will be subjected to a step-imposed heat flux from a semitransparent thin-film heater forming part of one wall of the container. Boiling is initiated and maintained for a defined period of time at a constant pressure level. Transient temperature measurements of the heater surface and throughout the fluid will be made. The boiling process is observed in two simultaneous views, from beneath the heating surface and from the side. The conduct of the experiment and the data acquisition will be completely automated and self-contained.

Task Significance:

The Pool Boiling Experiment (PBE) is designed to improve understanding of the fundamental mechanisms that constitute nucleate pool boiling. Nucleate pool boiling is a process wherein a stagnant pool of liquid is in contact with a surface that can supply heat to the liquid. If the liquid absorbs enough heat, a vapor bubble can be formed. This process occurs when a pot of water boils. On Earth, gravity tends to remove the vapor bubble from the heating surface because it is dominated by buoyant convection. In the orbiting space shuttle, however, buoyant convection has much less of an effect because the forces of gravity are very small. The Pool Boiling Experiment was initiated to provide insight into this nucleate boiling process, which has many Earth bound applications, such as steam-generation power plants, petroleum, and other chemical plants. Also, by using the test fluid R-113, the Pool Boiling Experiment can provide some basic understanding of the boiling behavior of cryogenic fluids without the large cost of an experiment using an actual cryogen.

Progress During FY 1996:**The Pool Boiling Experiment Has 5 Successful Flights:**

The experiment was conceived by Professor Herman Merte of the University of Michigan, developed at the NASA Lewis Research Center, and is supported by NASA Headquarters Microgravity Science and Applications Division. The pool boiling prototype system, which was initially flown on STS-47 in September 1992, acquired a considerable amount of scientific data. The expected boiling pattern was observed in all high-heat-flux cases, but a different pattern was observed in the low-heat-flux cases. These differences appear to be caused by the rewetting of the heater surface. The film data indicate that the saturated cases experienced a more activated boiling process (more vapor than expected was generated).

Some minor modifications were made in the timing sequences in the test matrix on the next two experiments which were flown on space shuttle flights STS-57(June 93) and STS-60(Feb 94). This was done to increase the probability of observing the initial dynamic vapor bubble growth while the camera was running at the higher speed and to observe the influence of a stirrer on the active boiling process. The results indicate the potential for quasi-steady nucleate pool boiling in long-term microgravity, with certain combinations of heat flux and bulk liquid subcooling. These were the first experiments of nucleate boiling obtained for long periods of microgravity, and the matrix test conditions were selected in part to cover the reasonably broad range of parameters.

The primary objective of the last two experiments, flown on STS-72(Jan 1996) and STS-77(May 96) was to determine the factors governing the onset of dryout and/or rewetting on a flat heater surface. On the STS-72 mission the subcooling levels were increased, while on the STS-77 mission the heat flux levels were reduced. For high heat flux levels, at all but the highest subcooling, dryout was observed. For lower levels of heat flux where dryout did not take place, it appeared that the excess surface energy associated with the coalescence of bubbles was sufficient to impel the resulting combined bubble away from the vicinity of the heater surface. This was sufficient to stir the liquid so as to bring the subcooled liquid to the heater surface.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	1
PhD Students:	2	PhD Degrees:	2

TASK INITIATION: 2/90 EXPIRATION: 12/96

PROJECT IDENTIFICATION: 963-24-0B-10

NASA CONTRACT NO.: NAG3-168

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Lee, H.S., Merte, H., Jr., Spherical vapor bubble growth in uniformly superheated liquids. Int. J. Heat Mass Transfer, (1996).

Lee, H.S., Merte, H., Jr., Hemispherical vapor bubble growth in microgravity: experiments and model. Int. J. Heat Mass Transfer, (1996).

Merte, H., Jr., Lee, H.S., Homogeneous nucleation in microgravity at low heat flux: experiments and theory. J. of Heat Transfer., (1996).

Presentations

Lee, H.S., and Merte, H., Jr., "The origin of the dynamic growth of vapor bubbles associated with vapor explosions." 1996 ASME International Congress and Exposition, in Atlanta, GA, for session "Nov. 17-22, 1996.

Lee, H.S., Merte, H., Jr., and Chiaramonte, F., "The pool boiling curve in microgravity." AIAA conference in Reno, NV, January 15, 1996.

Merte, H., Jr., "An overview of the microgravity environment and its effects on science." presented at AIAA 34th Aerospace Sciences Meeting, AIAA Paper 96-0401, Jan. 15-18, 1996, Reno, NV.

Merte, H., Jr., Lee, H.S., "Homogeneous nucleation in microgravity at low heat flux: experiments and theory." presented at Symposium "Heat Transfer in Microgravity Systems, 1995 International Mechanical Engineering Congress and Exposition" ASME Paper 95-WA/HT-41, San Francisco, CA, Nov. 13-17, 1995.

II. MSAD Program Tasks — Flight Research

Surface Tension-Driven Convection Experiment (STDCE-1, STDCE-2)

PRINCIPAL INVESTIGATOR: Prof. Simon Ostrach

Case Western Reserve University

CO-INVESTIGATORS:

Case Western Reserve University

Kamotani, Y.

Task Objective:

The objective of this research is to further the understanding of the physical mechanisms associated with non-oscillatory (STDCE-1) and oscillatory (STDCE-2) thermocapillary flow by (a) developing an accurate description of the physical mechanisms, (b) developing an accurate numerical model, and (c) obtaining ground-based and flight experimental data to verify the physical mechanisms and the numerical model. The thermocapillary flows result from the fluid motions generated by the surface-tractive force that is caused by surface-tension variation due to the temperature gradient along the free surface.

Task Description:

STDCE-1: The basis of Surface-Tension-Driven Convection Experiment 1 (STDCE-1) flight experiment is a copper test cell 10 cm in diameter and 5 cm deep, filled with silicone oil, able to provide both flat and curved free surfaces in a microgravity environment. The outer wall of the test cell is water cooled. The silicone oil can be centrally heated either externally by a carbon dioxide laser (constant heat flux, CF) or internally by an immersion heater (constant temperature, CT). The cross section is illuminated by a 1-mm-thick sheet of light, which scatters from small aluminum oxide particles mixed into the oil, allowing observation and measurement, using a particle-tracking technique, of the axisymmetric flow velocity. An infrared imager is used to measure surface temperature, and thermistors are used to measure fluid and wall temperature. The velocity and temperature measurements are compared with the numerical predictions.

STDCE-2: The center of Surface-Tension-Driven Convection Experiment 2 (STDCE-2) is an interchangeable module containing a test cell and fluid reservoir. Six modules containing copper test cells of 1.2, 2.0 and 3.0 cm diameter, each with the depth equal to the radius, will be filled with 2 centistoke silicone oil, to provide both flat and curved free surfaces in a microgravity environment. In three of the modules, one of each size, the fluid will be heated by a carbon dioxide laser, imposing a Gaussian heat flux on the free surface, and in the remaining three the fluid will be heated internally by an axially located heater which is ten percent of the chamber diameter. The outer walls of the test chambers will be cooled. This modular approach was taken to accommodate the large test matrix.

During the experiment, the surface temperature—which is the driving force in the flow—is measured non-intrusively by an infrared imager. The free-surface deformation, felt to play a critical role in the oscillation phenomenon, is measured quantitatively using a Ronchi deflectometer. The flow field is observed by illuminating the entire test chamber volume with laser light which is scattered from 20 micron aluminum oxide particles mixed in the fluid, allowing for three-dimensional qualitative visualization. Thermistors are used to measure bulk fluid, wall and heater temperatures.

At the start of each test the heater power will be slowly increased until the flow transitions from steady and axisymmetric to periodic and three dimensional. This will be performed for 43 combinations of test chamber size, heating mode and free surface shape. The temperature difference at the transition point will be used to calculate non-dimensional parameters which are used to characterize the onset of oscillations. The flow field, surface and bulk temperature distributions, and the free surface deformations will be correlated to support verification of the proposed physical mechanism for the oscillatory phenomenon.

Task Significance:

The Surface Tension Driven Convection Experiment is designed to study the nature and extent of steady and oscillatory thermocapillary flows using state of the art diagnostics to measure and characterize these flows over a wide range of parameters. Valuable data, which can only be gained from low gravity-based experimentation, will be obtained resulting in an understanding of the fundamental physical mechanisms and improved implementation of related industrial processes such as life support systems, containerless processing of materials, crystal growth, propellant storage management, and bio-fluids engineering both in space and on Earth.

Progress During FY 1996:

STDCE-1

STDCE-1 was flown on USML-1 in June 1992. 38 tests were completed returning over 12 1/2 hours of data. To date approximately 75% of the data has been analyzed and compared to the numerical model. The comparisons shown good agreement. This represents the relevant data from the experiment. The analysis of the data has been broken into sections and numerous presentations of those sections of the reduced flight data have been made. These include flow data from the 1 hr CT and CF tests, temperature data from the 1hr tests, flow data from the shorter CT flat surface tests, and flow data from the shorter CF curved surface tests. All of the reduced data has been compiled by a graduate student for the final contract report. In addition, no flow oscillations were observed in any of the tests corroborating the Principal Investigator's theory that the Marangoni number alone is not sufficient to indicate the onset of oscillatory flow.

The STDCE final report has been submitted and published as a NASA Contractor Report.

STDCE-2

Ground-based Work:

Investigations into the oscillation phenomenon were continued. The effect of buoyancy on the phenomenon was studied. Some investigators think that buoyancy is the reason why Marangoni number cannot correlate the experimentally determined onset conditions of oscillatory flow. This work clearly showed that buoyancy cannot explain that fact and has recently been accepted for publication in the Journal of Thermophysics and Heat Transfer (Kamotani, Masud, and Pline, 1996). In any case, other investigators are trying to find various reasons other than surface deformation to explain the above fact. For that reason, the floating zone configuration has been revisited because much data taken both in 1-g and micro-g are available for the oscillation configuration in that configuration. The objective was to show convincingly that the various factors mentioned by other investigators cannot explain the above fact and thus free surface deformation must be taken into account. This work has been accepted for publication in the Journal of Thermophysics and Heat Transfer (Masud, Kamotani, and Ostrach).

Flight Experiment:

The STDCE-2 experiments were conducted aboard the USML-2 Spacelab during its mission from October 20 to November 5, 1995. The experiments were very successful. All of the pre-mission defined tests as well as some additional tests were conducted. In all, 54 tests were conducted in the STDCE-2. The experiments were controlled and monitored at the NASA Marshall Space Flight Center in the Payload Operations and Control Center in Huntsville, Alabama. The interactive operation was very useful and many interesting phenomena were found as a result. 120 Hi-8 video tapes and 97 megabytes of digital data were returned. The quality of all the data was excellent.

In the STDCE-2 tests, the cold wall temperature stayed around 14 C, lower than typical wall temperatures in ground-based tests (about 25 C). Therefore, many ground-based tests are being repeated with the wall temperature kept near 14 C.

All of the data from the STDCE-2 have been received and are currently being analyzed. Testing to determine the accuracy of heater temperature measurements in the CT tests using the flight test chambers has been completed. It was found that the actual heater shell temperatures are smaller than the measured values during the flight. The differences in terms of DT (temperature difference) are about 30% for the 1.2 cm heater and 10% for the 2 and 3 cm heaters.

The software THERMAGRAM to analyze the IR Imager data, was received. Therefore, all the tools for the data analysis have been acquired. With the software all the IR Image data is being recorded in color for the convenience of data analysis.

After preliminary analysis of the STDCE-2 data, it is clear that the free surface deformation concept of oscillation mechanism is correct.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 4/91 EXPIRATION: 3/98

PROJECT IDENTIFICATION: 963-25-0D-09

NASA CONTRACT NO.: NAG3-156

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Kamotani, Y., Chang, A., and Ostrach, S., Effects of heating mode on steady axisymmetric thermocapillary flows in microgravity. *Journal of Heat Transfer*, vol. 118, pp. 191-197 (1996).

Kamotani, Y., Masud, J., and Pline, A., Oscillatory convection due to combined buoyancy and thermocapillarity. *Journal of Thermophysics and Heat Transfer*, vol. 10, pp. 102-108 (1996).

Kamotani, Y., Ostrach, S., and Pline, A., A thermocapillary convection experiment in microgravity. *Journal of Heat Transfer*, vol. 117, (November 3, 1995).

Lin, J. Kamotani, Y., Ostrach, S., An experimental study of free surface deformation in oscillatory thermocapillary flow. *Acta Astronautica*, vol. 35, (November 18, 1995).

Masud, J., Kamotani, Y., and Ostrach, S., Oscillatory thermocapillary flow in cylindrical columns of high prandtl number fluids. *Journal of Thermophysics and Heat Transfer*, (1996).

NASA Tech Briefs

Ostrach, S. and Kamotani, Y., Surface tension driven convection experiment (STDCE), NASA Contractor Report 198476. NASA Tech Brief, (June 1996).

Presentations

Kamotani, Y., Ostrach, S., and Pline, A., "Some temperature field results from the thermocapillary flow experiment aboard USML-2 spacelab." presented at the 31st Scientific Assembly of COSPAR, Birmingham, England, July 14-21, 1996.

Ostrach, S., "Surface tension driven convection experiment." presented at the 27th AIAA Fluid Dynamics Conference, New Orleans, LA, June 17-20, 1996.

Ostrach, S. and Kamotani, Y., "Surface tension driven convection experiment-2." Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 13-15, 1996.

Ostrach, S., Kamotani, Y., and Pline, A., "Oscillatory thermocapillary flows." presented at Fluids in Space, Naples, Italy, April 22-26, 1996.

Behavior of Rapidly Sheared Bubbly Suspensions

PRINCIPAL INVESTIGATOR: Prof. Ashok S. Sangani

Syracuse University

CO-INVESTIGATORS:

Koch, D. L.

Cornell University

Task Objective:

The objective is to test the average equations of motion governing bubbly suspension in an ideal setting where potential flow of continuous phase around bubbles prevails. To accomplish this, a microgravity experiment will be performed where a bubbly suspension is sheared in a couette cell and where the bubble volume fraction and velocity distribution are measured experimentally.

Task Description:

The proposed research has two aspects: The first of which is theoretical/numerical, and the second is experimental. Under the theoretical/numerical aspect the following work is planned:

- Development of a kinetic theory for bubbly suspension subjected to a simple shear motion. This theory will enable the expression of the overall dispersed phase stress in terms of a mean rate of strain tensor. This established rheology will be combined with the dispersed phase stress due to relative motion of bubbles with respect to the liquid flow under gravity.
- Analysis of the stability of bubbly suspension in the presence of simple shear and mean relative motion induced by buoyancy force acting on the bubbles.
- Numerical simulation of bubbly suspension subject to shear in microgravity as well as under full gravity. A new method/algorithm based on the fast multiple expansion technique will be developed and will allow simulation of large number of bubbles (104-105), and this large number is needed to detect instabilities in the suspension.

Under the experimental aspect of this work, the following is proposed:

- Perform an experiment involving cylindrical couette flow of a bubbly suspension in the microgravity environment. The motion of the bubbles will be solely determined by the centrifugal force which tend to push the bubbles toward the inner cylinder. The shear flow will drive bubble collision and create a bubble pressure that resists the accumulation of bubbles. After an elapsed period of time, a steady state volume fraction profile will develop. By measuring the variation of bubble volume fraction and bubble and liquid velocities across the gap of the couette, the average equations of motion can then be tested. As a subset of this experiment, several experiments performed under ground and reduced gravity conditions will be performed to support the development of the flight experiment.

Task Significance:

This work will result in the fundamental understanding of bubbly suspension behavior in a well controlled environment where gravity is not present and under potential flow conditions. A better understanding of this behavior affects the design of industrial processes that require using bubbly suspensions. Chemical, petroleum, and pharmaceutical processes are examples of industrial processes that involve bubbly suspensions.

Progress During FY 1996:

A kickoff meeting was held on June 17, 1996 during which the Principal Investigator and Co-Investigators presented the scope of work and the experiment objective and theory. A Quality Functional Deployment team was formed to assess the feasibility issues of the project. The team formulated its report on this flight definition experiment which addressed the science, engineering, and timelines of the experiment.

PIs are in the process of procuring the hot wire probes which will be used to measure the volume fraction and velocity distribution in the couette. These probes will be tested in a bubbly suspension flow in an inclined plane setting.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 5/96 EXPIRATION: 4/00

PROJECT IDENTIFICATION: 963-25-OH

NASA CONTRACT NO.: NAG3-185

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Kang, S.Y., Sangani, A.S., Tsao, H.K., and Koch, D.L. Rheology of dense bubble suspensions. Physics o Fluids, (submitted, 1996).

Modeling and New Experiment Definition for the VIBES

PRINCIPAL INVESTIGATOR: Prof. Robert L. Sani

University of Colorado, Boulder

CO-INVESTIGATORS:

Azuma, H.

Japanese National Aerospace Laboratory (NAL)

Doi, T.

NSDA — Japanese Space Agency

Kamei, S.

Mitsubishi Research Institute

Ohnishi, M.

Japanese National Aerospace Laboratory (NAL)

Kida, T.

Japanese National Aerospace Laboratory (NAL)

Yamamoto, K.

Japanese National Aerospace Laboratory (NAL)

Task Objective:

The Vibration Isolation Box Experiment System (VIBES) is an IML-2 flight experiment designed by the Japanese National Aerospace Laboratory. Its primary goal is to evaluate the performance of a vibration isolation device in conjunction with typical fluids experiments. The IML-2 flight experiment contains two experimental units: the Convection Diffusion Unit (CDU) and the Thermal-Driven Flow Unit. The purposes of the CDU experiment (the one of interest herein) are to observe natural convection and diffusive transport in a micro-g environment and to observe the effect of g-jitter with and without the vibration isolation due to the vibration isolation box. The objective of this project is to provide numerical modeling for the CDU experiment for aiding in design refinements and evaluation of terrestrial benchmark experiments as well as post-flight evaluation of the experimental data.

Task Description:

The numerical modeling will utilize a Galerkin finite element algorithm for the linear momentum, energy and species balance equations using the Boussinesq approximation. This project will make comparisons of two codes (PI's research code and a commercial code, FIDAP) in a transient, 3-D calculation to determine their efficiency and accuracy. Timing comparisons will also be made between FIDAP and the research code. The numerical experiments will include example cases with and without the test cell being subjected to g variation; both single and multiple frequency variations will be considered. The numerical experiment will also consist of simulating the g-environment (to be provided by the Japanese research team) both inside and outside the isolation box. Comparison of these results should allow a quantitative assessment of the isolation capability of the apparatus.

Task Significance:

The microgravity environment available for space experiments is not quiescent but is subjected to significant background vibrations generated by aerodynamic and machinery vibrations, crew motion, etc. Such g-jitter can be relatively random in orientation and can attain significant magnitudes. There is a growing list of observations and data analyses that demonstrate the existence of significant g-jitter episodes and their potential for having very deleterious effects on many proposed flight experiments. A potential solution to this problem in the micro-g environment is the use of vibration isolation for the experiments which require it. The assessment of such an apparatus is one of the main thrusts of the research proposed in this project.

Progress During FY 1996:

This MSAD-funded research project is to provide numerical modeling of the VIBES (Vibration Isolation Box Experiment System) which was an IML2 flight experiment built by the Japanese research team of Dr. H. Azuma of the Japanese National Aerospace Laboratory and was successfully conducted on the IML2 mission. In addition to the modeling of the VIBES experiment general modeling capability is being developed for preflight experiment design of contained flow systems subjected to thermal and multiple specie fields. During this final reporting period, two main areas, model development and flow simulation, have been addressed:

I. MODEL DEVELOPMENT

In order to improve the capability of the numerical algorithm to model convective transport effects a skew-symmetric form of the advective transport term has been implemented and successfully tested. In conjunction

with this implementation a bi-conjugate gradient stabilized solution algorithm has been incorporated to facilitate the solution of the asymmetric system of equations which the skew-symmetric form generates when incorporated into our semi-implicit solution scheme. During this reporting period we have demonstrated the effectiveness of this scheme in advection dominated flows and transport. The algorithm has also been modified to facilitate the incorporation of additional fields, such as multiple species, which could become an issue when addressing other problems.

2. TIME-VARYING BOUSSISNESQ FLOW SIMULATIONS

Simulation of ground based experiments with a time varying gravitational field have been extended from those done during the last reporting period to validated our model as well as provide some fundamental insight into such processes. In addition some scenarios which were suggested by the results of the VIBES experiment have been addressed.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 1/93 EXPIRATION: 1/96

PROJECT IDENTIFICATION: 963-24-05-14

NASA CONTRACT No.: NAG3-141

RESPONSIBLE CENTER: LeRC

Studies in Electrohydrodynamics

PRINCIPAL INVESTIGATOR: Dr. Dudley A. Saville

Princeton University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This research is designed to strengthen and test the experimental foundations of the theory of electrohydrodynamics. Electrohydrodynamic forces can be used to manipulate fluids, especially fluid interfaces. As such, they offer a means of controlling fluid motion on very small length scales.

Task Description:

Theoretical studies will center on adapting the existing leaky dielectric theory for the stability of a fluid cylinder to account for pinning the contact line at the upper and lower boundaries in a liquid bridge configuration. Experimental studies will be carried out to (1) evaluate the influence of ionic surfactants on conductivity so as to enable us to control the time scale of the electrohydrodynamic fluid motion and (2) test the existing electrohydrodynamic theory for the stability of a cylinder subject to an axial field with isopycnic systems. A successful series of experiments were carried out on the June 1996 LMS mission. In the LMS experiments, fluids cylinders deployed in a gas were stabilized against the capillary instability by both DC and AC electric fields.

Task Significance:

Despite substantial efforts over the past two decades, the foundation of electrohydrodynamics is weak. Relatively few experiments have been done to test the leaky dielectric theory, the most promising model of behavior, and much of the work has been of limited scope because of the need to use isopycnic systems to avoid sedimentation and hydrostatic pressure effects. This restricts the range of fluid properties that can be studied and as a result there are many gaps in our knowledge. In addition to its scientific importance, there are a wide range of applications where electrohydrodynamic phenomena play important roles.

Progress During FY 1996:

In June of 1996 a very successful flight experiment was carried out on the LMS mission aboard the Columbia space shuttle. This experiment was conducted in collaboration with the European Space Agency (ESA) with the apparatus constructed and tested under the auspices of ESA. The elapsed time from the "science concept review" to flight was just over eighteen months, demonstrating that it is possible to complete a significant space experiment in a relatively short time frame. Over thirty-six hours of interactive experiments were carried out using both ac and dc fields with voltages up to 20 kV. From mechanical and electrical points of view everything worked better than anticipated. The scientific results are currently being analyzed.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 1

TASK INITIATION: 4/93 EXPIRATION: 7/97

PROJECT IDENTIFICATION: 963-25-10

NASA CONTRACT NO.: NAG8-969

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Lempert, W.R., Harris, S.R., Hersch, L., Burcham, C.L., Miles, R.B., Gee, K., Haugland, R.P., and Saville, D.A.
"Quantitative flow visualization of internal circulation in droplets by phantom flow tagging." American Institute of Aeronautics and Astronautics, 1995 AIAA Meeting, Paper AIAA-95-0168, Reno Nevada, January 1996.

Mechanics of Granular Materials

PRINCIPAL INVESTIGATOR: Dr. Stein Sture

University of Colorado, Boulder

CO-INVESTIGATORS:

Costes, N.

NASA Marshall Space Flight Center (MSFC)

Task Objective:

The objective of this research is to gain a quantitative understanding of the mechanical behavior of cohesionless granular materials under very low effective confining pressures.

Task Description:

Ground-based displacement-controlled triaxial experiments are conducted on a cohesionless granular material at the lowest effective confining pressures possible, that do not result in material instability, to assess constitutive properties, stability phenomena, and control parameters that will be applied to in-space experiments on 75 mm (diameter) and 150 mm (length) right cylindrical specimens. The ground-based tests on similar-sized specimens are conducted in the range 3.5-69 kPa, while the microgravity tests will be conducted at effective confinement levels in the range 0.05-1.30 kPa.

The displacement-controlled mode of loading confined specimens was chosen mainly to maintain overall specimen-apparatus stability while strain-softening resulting from continuous or discontinuous bifurcation and discontinuous deformation fields are allowed to take place. Optical and other noncontacting displacement-sensing techniques are used to measure specimen response during experimentation. Prescribed displacements are transmitted in terms of loading, unloading, and reloading histories, while volume change is measured in "drained" tests, and pore fluid pressure is measured in "undrained" isochoric tests. Confinement pressure is transmitted to the granular material assembly through a thin flexible latex membrane surrounding the specimen. A subangular and uniform Ottawa quartz sand constitutes the specimen.

Specimens tested both in space and on ground will be subjected to nondestructive and destructive (thin-slicing) testing to assess degrees of material uniformity and isotropy before and after experimentation. It appears that instability phenomenon associated with specimens of certain configurations result in curved internal surfaces of localized deformation and high rates of dilatancy, whose structure depends on bifurcation mode.

Task Significance:

Specifically, the purpose is to study the influence of particle interlocking and other fabric properties on the strength criterion near the effective stress space origin, i.e., can it be represented by a straight-line envelope passing through the origin or does it have a curved shape with shear (cohesion or interlocking) or tensile strength intercepts. The experiment will determine whether cohesionless granular materials under very low effective confining pressures/effective stresses tend to dilate or contract regardless of their initial state of compaction, and whether their mechanical behavior under relatively large displacement or quasi-static cyclic loading is according to conventional constitutive theory. In addition, bifurcation and material instability phenomena resulting in formation of shear bands, before and after peak strengths have been reached, will be studied. Based on terrestrial experiments and theory, it has been found that critical hardening, strain-softening behavior, and shear band orientation are dependent on confining stress.

Progress During FY 1996:

The progress in the MGM project during FY95 includes the following:

1. Completion and testing of the MGM apparatus;
2. Improved analysis of tested specimens;
3. Training of payload/mission specialists;
4. Improved constitutive models;
5. Improved analysis of specimen bifurcation instability conditions; and,
6. Improved optical-imaging and measurement systems.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1 BS Degrees: 1
MS Students: 1 MS Degrees: 1
PhD Students: 2 PhD Degrees: 1

TASK INITIATION: 12/92 EXPIRATION: 9/97

PROJECT IDENTIFICATION: 963-55-05

NASA CONTRACT No.: NAS8-387

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Larsson, R., Runesson, K., and Sture, S. Embedded Localization Band in Undrained Soil Based on Regularized Strong Discontinuity - Theory and FE analysis. Int. J. Solids and Structures, vol. 33, no. 20, 3081-3101 (1996).

Runesson, K., Peric, D., and Sture, S. Effect of Pore Fluid Compressibility on Localization in Elastic-Plastic Porous Solids under Undrained Conditions. Int. J. Solids and Structures, vol. 33, no. 10, 1501-1518 (1996).

Proceedings

Costes, N.C., and Sture, S. "Issues on geomechanics." Proceedings of the ASCE 5th International Conference on Space '96, pp 516-520, Albuquerque, New Mexico, 1996.

Thermocapillary Migration and Interactions of Bubbles and Drops

PRINCIPAL INVESTIGATOR: Prof. R. S. Subramanian

Clarkson University

CO-INVESTIGATORS:

Balasubramaniam, R.
Wozniak, G.

NASA Lewis Research Center (LeRC)
Tu Bergakademie Freiberg (Germany)

Task Objective:

The objectives of the research are to experimentally measure, both in one-g and low-g, the thermocapillary migration velocities and the shapes of single and interacting gas bubbles and liquid drops in a continuous phase under the action of an applied temperature gradient. Comparisons between the observed velocities and shapes with those that are predicted from theory will be made. The low-g results will bear data that will be free from the effects of buoyant convection in the continuous phase as well as buoyancy effects on the bubbles/drops themselves.

Specific objectives differed for these LMS experiments when compared to the experiments conducted for the IML-2 mission. It was the intent for the LMS experiments to: focus on the interactions of pairs of bubbles or drops (the IML-2 mission focused on isolated bubbles and drops); study velocity distributions around bubbles using tracer particles illuminated by light sheets; as well as studying isolated bubbles and drops again but at higher Marangoni and Reynolds numbers, and lower Marangoni numbers as well.

Task Description:

The general approach has been to conduct ground-based normal-gravity testing and to develop theoretical models of the thermocapillary migration phenomena. The instrumentation and diagnostics are centered on the physics of interest, namely, flow fields, temperature fields, and bubble/droplet velocities and shapes. The predictions developed and verified with the one-g data will be used to design and predict the results of the flight experiments. In addition, for this reporting period, the flight data from the IML-2 experiments was used and is being used to construct improved models for both bubbles and drops. LMS preparatory as well as mission activities and results will be reported on below.

Task Significance:

The results from these bubble migration experiments are not only expected to advance our knowledge in the area of surface tension driven motion, but are, in addition, relevant to several applications with respect to space processing of materials. Some examples of the latter include solidification, glass processing, and composite preparation. The physics studied in these experiments offer a method by which the risk of getting undesirable voids (gas pockets) in the formation of metals and composites can be minimized.

Progress During FY 1996:

Efforts in FY 96 were four-fold: 1) continuing the analysis of their IML-2 flight data; 2) continuing the preparation for the LMS mission; 3) conducting experiments during the LMS mission; and 4) analyzing LMS flight data. Concerning point 1), the video and film images have been analyzed for bubble and droplet speeds (as previously reported). In addition, the modeling of the isolated bubble migrations (as previously reported) and the modeling of the isolated droplet migrations (for large Marangoni numbers) has now been done. Experimental results showed good agreement with theoretical predictions in the case of isolated bubbles. There were some discrepancies, however, at the lower Marangoni numbers. Explanations for this could be because the viscosity is a function of temperature over the ranges studied, and due to wall effects on the thermal fields. Some simplified modeling has been done for interacting bubble pairs and has showed some qualitative agreement with the IML-2 data.

Concerning point 2), there were several changes made to the test cell in evolving from IML-2 to LMS experiments. The continuous phase fluid's viscosity was lower for LMS (10 cS versus 50 cS). Tracer particle technology (in conjunction with laser light sheeting) was used in the bubble test container to be able to gather data on the external velocity fields. A shearing interferometric system (Wollaston prism interferometry) was implemented in the BDPU facility, at the suggestion of the PI team, to gather data on the external thermal fields surrounding bubbles and

drops. This was seen to work best for temperature differences less than 30 degree-C. Dissolution of the droplet material (FC-75) into the silicone oil was also brought up as a concern. This would have affected the thermal data near the interface.

Tests were conducted at the PI site and this effect turned out to be small, however. In addition, there were the normal sorts of necessary pre-mission activities such as mission simulations at MSFC, validation tests at contractor sites, and the requisite document preparation.

Concerning point 3), as previously mentioned these LMS experiments focused on the thermal migration of pairs of drops and pairs of bubbles in a continuous phase liquid. It was also planned to conduct isolated bubble and drop runs at high and low Marangoni numbers to complement the IML-2 data. The LMS experiments were done in four stages alternating between the bubble and droplet test containers. These experiment durations were 19.9 hrs (first bubble), 15.5 hrs (first drop), 21.2 hrs (second bubble), and 5.0 hrs (second drop). Video, film (cine), interferometry, and light sheet tracer data was taken throughout these experiments. The Wollaston Prism Interferometer yielded good quality data. Experiment operations were hampered by occasional sparse real time TV coverage due to non-optimal shuttle orientations.

Concerning point 4), the analyses of the video, film, and digital data continues and will go on for some time hence.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	2
PhD Students:	1	PhD Degrees:	2

TASK INITIATION:	1/90	EXPIRATION:	6/97
PROJECT IDENTIFICATION:		963-25-0C-61	
NASA CONTRACT NO.:		NAG3-112	
RESPONSIBLE CENTER:		LeRC	

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Balasubramaniam, R. and Subramanian, R.S. Thermocapillary bubble migration - Thermal boundary layers for large Marangoni numbers. *Int. J. Multiphase Flow*, vol. 22, no. 3, 593-612 (1996).

Balasubramaniam, R., Lacy, C.E., Wozniak, G., and Subramanian, R.S. Thermocapillary migration of bubbles and drops at moderate values of the Marangoni number in reduced gravity. *Physics of Fluids*, vol. 8, no. 4, 872-880 (1996).

Drop Dynamics Investigation

PRINCIPAL INVESTIGATOR: Prof. Taylor G. Wang

Vanderbilt University

CO-INVESTIGATORS:

Lee, C.P.

Anilkumar, A.V.

Hmelo, A.B.

Hussein, H.J.

Daidzic, N.

Vanderbilt University

Vanderbilt University

Vanderbilt University

Vanderbilt University

Vanderbilt University

Task Objective:

The objective of this program is to understand the behavior of free liquid drops, primarily by studying them in a microgravity environment. The Drop Physics Module (DPM) operated in the Space Shuttle provides an opportunity to address outstanding fluid-dynamics issues of rotating and oscillating simple and compound drops. To maximize the return from this short on-orbit opportunity, ground-based experiments will be performed to verify concepts and experimental techniques, and modeling will be done to select the parameters for the DPM experiments.

This investigation will use a triple-axis acoustic positioning chamber to study the static shape and the dynamics of simple and compound drops. Equilibrium shapes and the stability of rotating and nonrotating drops, their associated internal flow patterns, and the centering force associated with shape oscillations of compound drops—will be the principal scientific areas of interest.

Task Description:

A variety of experiments will be performed in space. Compound drops and liquid shells were formed to study their oscillation modes and the effectiveness of those modes in centering the core. The interaction between the acoustic field and the drops were studied: the drops' static shape, the stability of distorted shapes, and the generation of any flows in the drops. The dynamics and stability of rotating drops near the point of fission will be explored.

Task Significance:

This investigation uses the low gravity provided by the Space Transportation System, the working laboratory of Spacelab, and the Drop Physics Module hardware to study large drops. Studying drops of size 1-3 cm. in diameter shows dynamic phenomena to time scales, which can be observed by the experiment operator (video) as well can be captured on high-speed film.

Progress During FY 1996:

Preliminary results from USML-2 show that acoustic flattening has strong influence on the bifurcation process. For small levels of flattening, bifurcation occurs at lower rotation rates, in accordance with the earlier results. As flattening increases, the bifurcation point shifts farther. Beyond a certain level of flattening, rotation affects the equilibrium of the drop and the classical bifurcation route is not followed. This result, along with the data on the shift in bifurcation point with flattening, should stimulate theoretical work in this area.

During USML-2, oscillation-induced centering was studied in immiscible compound drops of large shell-core volume ratios (>4). Preliminary results for such drops show that the coupling of the oscillations in the bubble-mode are weak, and thereby no centering could be effected in the bubble-mode. On the contrary, the compound drop could be driven to large amplitudes in the slosh mode and centering could be effected.

Preliminary study of the video tapes at Vanderbilt University - Center for Microgravity Research and Applications recorded at the ground station in MSFC (via HIPAC system) showed clear evidence of transition from periodic to chaotic drop oscillations. Multifrequency excitation has proved to be a suitable and efficient tool to bring drop quickly into chaotic oscillations without excessive amplitudes and by preserving the levitation stability. Physically, the transition to chaos is enabled through the ultrasubharmonic resonance and forced period-coupling (frequency is halved). This first period-doubling is then responsible for the subsequent period-doubling bifurcations and quick transition into chaotic (noise-like) oscillation regime.

Flight verification of tumble rotation mechanism during USML-2 is obtained by measuring the slope of the velocity vs time curve is -0.068 sec^{-2} . If we consider the drop as a solid body and use the moment of inertia for a drop of the deployed size shape and density, we can determine the torque that was responsible for the deceleration. This is found to be $0.10 \pm 0.01 \text{ dyne-cm}$, in good agreement with our ground based estimates.

Theoretical studies of the following six subjects are underway:

1. The effects of acoustic flattening of the $n=2$ rotational bifurcation of a drop
2. The effects of rotation on the equilibrium of an acoustically flattened drop
3. Dynamic fission of a drop after losing stable equilibrium, at the end of the $n=2$ bifurcation path due to rotation
4. Centering of a liquid-core compound from of finite volume ratio in large amplitude oscillations
5. Multi-frequency excitations of drop oscillations, looking for development of chaos
6. Frequency sweep in excitation of a drop, looking for hysteresis and jump phenomenon.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	3	MS Degrees:	2
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 8/92 EXPIRATION: 7/96

PROJECT IDENTIFICATION: 963-24-04-01

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Hmelo, A.B., Battaile, C.C., and Wang, T.G. The velocity of sound in liquid succinonitrile near the melting temperature. Journal of Acoustical Society of American, (in press).

Shen, X.F., Anilkumar, A.V., Grugel, R.N., and Wang, T.G. Utilizing vibration to promote microstructure homogeneity in crystals during floating-zone processing. J. Crystal Growth, in press, (1996).

Wang, T.G., Anilkumar, A.V., and Lee, C.P. Oscillations of liquid drops: Results from USML-1 experiments in space. J. Fluid Mech, vol. 308, 1-14 (1996).

A Study of the Constrained Vapor Bubble Heat Exchanger

PRINCIPAL INVESTIGATOR: Prof. Peter C. Wayner, Jr.

Rensselaer Polytechnic Institute

CO-INVESTIGATORS:

Plawsky, J.

Rensselaer Polytechnic Institute

Task Objective:

The objective of this effort is to better understand the physics of evaporation and condensation as they affect the heat transfer processes in a constrained vapor bubble heat exchanger (CVBHX). This CVBHX consists of a small enclosed container partially filled with a liquid. When a temperature difference is applied to the ends of the CVBHX, evaporation occurs at the hot end and condensation at the cold end — resulting in a very effective heat transfer device with great potential in space applications.

Task Description:

A near-term flight experiment concept will be developed to pursue both equilibrium and non-equilibrium testing of the CVBHX operation. Flight-qualified apparatus and optical instrumentations will be designed and developed. The microscopic intermolecular force (pressure) field, which is a function of the liquid film thickness profile, will be measured using microcomputer enhanced video microscopy based on interferometry. The augmented Young-Laplace equation over a large range of film thickness will be evaluated. The overall heat conductance of the CVBHX as a function of liquid volume and heat flow rate can also be determined.

Models of the transport processes in the contact line region of a CVBHX which include the effects of liquid-solid and liquid-vapor intermolecular forces have already been developed. As part of this effort, these models will be further refined and the transport characteristics of CVBHX's will be obtained by comparing the experimental data to numerical solutions of the model.

Task Significance:

This study is synergistic in that the space program needs passive systems like the CVBHX for thermal control and research on a CVBHX requires a microgravity environment. This study is also multi-faceted: (1) It is a basic study in interfacial physics because the CVBHX is used to measure the dispersion constant which characterizes the interfacial intermolecular force field; (2) It is a basic study in fluid physics because it evaluates fluid flow in ultra-thin liquid films; (3) It is a dynamic study in thermal transport because it evaluates the heat transfer capabilities of a small scale heat exchanger; and (4) The CVBHX can also be called a wickless heat pipe heat exchanger. The results from this study are not only applicable to space applications, but can also help the design of conventional heat pipes which are poorly understood.

Progress During FY 1996:

This is a new project which just started in April, 1996. The PI has been working closely with LeRC in-house evaluation team to define the science requirements, the technical requirements and the feasibility issues to prepare for the Phase-A work of this flight project.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 4/96 EXPIRATION: 4/00

PROJECT IDENTIFICATION: 963-25-OH

NASA CONTRACT NO.: NAG3-183

RESPONSIBLE CENTER: LeRC

Physics of Colloids in Space

PRINCIPAL INVESTIGATOR: Prof. David A. Weitz

University of Pennsylvania

CO-INVESTIGATORS:

Pusey, P.N.

The University of Edinburgh

Task Objective:

This experiment entails the study of the physics of colloidal particles in microgravity. It consists of two distinct parts. The first deals with ordered structures while the second deals with highly disordered structures. The study of ordered structures entails the growth of colloidal superlattices formed with mixtures of different-sized particles. The goal is to develop useful periodic structures using colloidal particles as precursors, through "colloid engineering." The study of the highly disordered structures entails the formation of fractal colloidal aggregates of much greater extent than has ever been done, and the formation of very weak structures that would collapse under their own weight in normal gravity.

Task Description:

The work within this effort is ground-based research to study the formation of novel materials from colloidal dispersions, and to study the physical properties of such materials. As part of the effort, space experiments to be carried out in a space shuttle middeck carrier, will be defined. These experiments will utilize the laser light scattering apparatus currently being developed at NASA LeRC.

The focuses of the ground-based experiments are the study of colloidal superlattices formed from mixtures of different-sized colloidal particles, the in-depth study of the formation of fractal colloidal aggregates. While considerable knowledge exists about the formation or growth of fractal colloidal aggregates, much less is known about the unique properties of these objects and the consequences of their scale invariance. A major reason for this is the relatively small scale over which the aggregates exhibit scale invariant behavior. By growing structures that are scale invariant over a much greater range of length scales, the properties of these objects can be studied much more directly. This will provide the first detailed information about the consequences of scale invariant structure on the properties of these materials.

The work within this effort is the ground-based research required to define experiments to be carried out on a space flight. These experiments will use the laser light scattering apparatus developed at NASA LeRC. Two glovebox experiments have been defined and prepared, one scheduled to fly on MIR in the fall of 1996, and the second scheduled to fly on MIR in 1997. In addition, ongoing work is aimed at defining a longer term experiment for the ISS.

The focus of the investigation is the study of colloidal superlattices formed from mixtures of different-sized colloidal particles, and the study of fractal colloidal gels made from colloidal aggregates and from mixtures of colloids and polymers. The colloidal superlattices are formed from binary alloy colloidal crystals, and the work aims to determine their phase behavior, crystal structure and growth properties. The colloidal gels are formed from fractal aggregates and this work allows the properties of these remarkable materials to be studied on detail. In addition, the study of the colloid-polymer mixtures probes the phase separation of coexisting mixtures of colloidal gas, liquid and crystals.

Task Significance:

Very little is currently known about the structures of binary colloidal crystals, and these experiments will initially be directed at determining the phase diagrams of the superlattices for mixtures of different sizes of particles. In addition, virtually nothing is currently known about the kinetics of the formation of these superlattices, and about their dynamics once they are formed. This will also be studied by these experiments. This will represent the first in-depth study of the growth and properties of colloidal superlattices.

II. MSAD Program Tasks — Flight Research

Progress During FY 1996:

This project successfully completed the Requirements Definitions Review(RDR). The final draft of the Science Requirements Document (SRD) was completed. It was proposed that PCS be supported by two Mir Space Station Glovebox missions. The first mission, the experiments on superlattice crystal formation in bidisperse colloid mixtures and gelation of colloid plus polymer mixtures, is tentatively scheduled for the September 1996 Mir flight. These experiments require PMMA colloidal particles. Initial difficulties with their synthesis have now mostly been overcome, although some problems remain in the preparation of highly monodisperse small particles. Enough monodisperse material was prepared to supply training and flight samples for the first proposed mission. A ground-based experiment was begun to see if superlattice structures form in zero-gravity as simulated by slow tumbling. A well developed theoretical understanding was attained for the behavior of density-matched polystyrene (PS) gels, as it has been observed in all experiments made to date. It is now possible to measure the elasticity of gels by an entirely optical technique. Development continued of the PCS in-software correlator, necessary for determining the behavior of PS gels in a regime currently inaccessible to measurements. More understanding was reached on the phase diagram and gelation kinetics of colloid plus polymer mixtures. With this system it will be possible to determine the consequence for gels of a flexible bond between particles, rather than the rigid bond of PS gels, but since the colloid plus polymer mixture system cannot be density-matched, a zero-gravity environment is essential for experiments. Training and flight samples were prepared for the first Glovebox flight. Emulsion droplets are likely to provide one of the components of future heterogeneous systems. Therefore, much work was done in order to understand the light-scattering, rheological, and crystal forming behavior of oil droplet emulsions. New techniques were developed for the emulsification of liquid crystals. These techniques may eventually be applied in the assembly of novel order materials in zero gravity.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 3/94 EXPIRATION: 3/97
PROJECT IDENTIFICATION: 963-24-05-13
NASA CONTRACT NO.: NAG3-185
RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Gang, H., Krall, A.H., and Weitz, D.A., Thermal fluctuations of the shapes of droplets in dense and compressed emulsions. *Phys. Rev. E*, 52, 6289-6302 (1995).

LaCasse, M.-D., Grest, G.S., Levine, D., Mason, T.G., and Weitz, D.A., A model for the elasticity of compressed emulsions. *Phys. Rev. Lett.*, 76, 3448-3451 (1996).

Ladd, A.J.C., Gang, H., Zhu, J.X., and Weitz, D.A., Temporal and spatial dependence of hydrodynamic correlations: simulation and experiment. *Phys. Rev. E*, 52, 6550-6572 (1995).

Liu, A.J., Ramaswamy, S., Mason, T.G., Gang, H., and Weitz, D.A., Anomalous viscous loss in emulsions. *Phys. Rev. Lett.*, 76, 3017-3020 (1996).

Mason, T.G. and Weitz, D.A., Linear viscoelasticity of colloidal hard sphere suspensions near the glass transition. *Phys. Rev. Lett.*, 75, pp. 2770-2773 (1995).

Mason, T.G., Bibette, J., and Weitz, D.A., Yielding and flow of monodisperse emulsions. *J. Colloid Interfac. Sci.*, 179, 439-448 (1996).

Mason, T.G., Krall, A.H., Gang, H., Bibette, J., and Weitz, D.A., Monodisperse emulsions: properties and uses. *Encyclopedia of Emulsion Technology*, P. Becher, Ed., vol. 4, 299 (1996).

Mason, T.G., Krall, A.H., Gang, H., Bibette, J., and Weitz, D.A., Monodisperse emulsions: properties and uses. *Encyclopedia of Emulsion Technology*, P. Becher, Ed., vol. 4, 299 (1996).

Page, J.H., Schriemer, H.P., Bailey, A.E., and Weitz, D.A., Experimental test of the diffusion approximation for multiply scattered sound. *Phys. Rev. E*, 52, 3106-3114 (1995).

Page, J.H., Sheng,P., Schriemer, H.P., Jones, I., Jing, X., and Weitz, D.A., Group velocity in strongly scattering media. Science, 271, 634-637 (1996).

Weitz, D.A., Materials: foams flow by stick and slip. Nature, 381, 476 (1996).

Weitz, D.A. and Ladd, A.J.C., Response to comment. Phys. Rev. Lett., 75, 2253 (1995).

Proceedings

Krall, A.H. and Weitz, D.A. "Dynamic Light Scattering from Colloidal Gels." Proceedings of the Third NASA Conference on Fluid Physics, NASA CP 3338, pp.403 & 407, Cleveland, OH, June 13-15, 1996.

Weitz, D.A., "Complex fluids: Science, technology and microgravity." Proceedings of the Third NASA Conference on Fluid Physics, NASA CP 3338, pp. 25-26, Cleveland OH, June 13-15, 1996.

Microgravity Test of Universality and Scaling Predictions Near the Liquid-Gas Critical Point of ^3He

PRINCIPAL INVESTIGATOR: Dr. Martin B. Barmatz

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Rudnick, J.

Hahn, I.

Israelsson, U.

University of California, Los Angeles

Jet Propulsion Laboratory (JPL)

Jet Propulsion Laboratory (JPL)

Task Objective:

The objectives of this task are to test the universality and scaling laws at the liquid-gas critical point of ^3He in a microgravity environment. The task objectives will include 1) precision measurements of the isothermal compressibility along the critical isochore to determine the critical exponent γ ; 2) precision measurements of the constant volume specific heat along the critical isochore to determine the critical exponent α ; and 3) precision measurements of the density dependence of the pressure along the critical isotherm to determine the critical exponent δ .

Task Description:

Theories describing the behavior of thermophysical properties near critical points were developed using the concept of scaling laws. These models led to the definition of universality classes where critical points of the same class are predicted to have the same critical exponents. Efforts to validate the scaling law predictions near a liquid-gas critical point in the ground-based laboratories are limited due to the gravity-induced vertical density gradient associated with the divergence of the isothermal compressibility. This density gradient becomes appreciable as the critical point is approached, leading to a significant smearing of the transition. Calculations have shown that in a microgravity environment (10^{-6} g) accurate specific heat and isothermal compressibility measurements could be obtained two orders of magnitude in reduced temperature closer to the critical point. These studies will require accurate measurements of pressure ($\Delta p/p \sim 10^{-11}$), density ($\Delta \rho/\rho \sim 10^{-9}$), and temperature ($\Delta T/T \sim 10^{-9}$). These simultaneous measurements in microgravity should provide a very stringent test of theoretical predictions.

Task Significance:

The ability to perform these simultaneous measurements should provide a very stringent test of the scaling predictions.

Progress During FY 1996:

This task was started late in FY 1996. Testing of the high resolution thermometers and of the density measuring capacitor is proceeding.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 963-31-00-00

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Barmatz, M., and Hahn, I. "Measurements near the liquid-gas critical point of ^3He ." Proceedings of the 21st International Low Temperature Physics Conference LT-21 (Prague), Czechoslovak Journal of Physics 46 (1996).

Barmatz, M. and Hahn, I. "Measurements near the liquid-gas critical point of ^3He ." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA Document D-13845 (1996).

Rudnick, J., and Barmatz, M. "Electric fields near the liquid-vapor critical point." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA Document D-13845 (1996).

Critical Dynamics in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Robert V. Duncan

University of New Mexico

CO-INVESTIGATORS:

Chui, T.C.P.
Israelsson, U.E.
Liu, Feng-Chuan

Jet Propulsion Laboratory (JPL)
Jet Propulsion Laboratory (JPL)
Jet Propulsion Laboratory (JPL)

Task Objective:

The nature of continuous (sometimes called 'second-order') transitions in systems driven well away from equilibrium is of fundamental scientific importance, yet not well understood. DYNAMX shall investigate such a system through measurements of the thermal gradients near the superfluid - normal fluid (He-II/He-I) interface while it is subjected to a heat flux Q in a microgravity environment. These thermal profile measurements shall be used to study the effective thermal conductivity very close to the interface where linear response has been predicted to fail, and to study dynamical effects on the interfacial thickness, and on the heat flux induced depression of the superfluid transition temperature. A second series of measurements shall be conducted on orbit to study heat flux effects on the heat capacity near the superfluid transition. Microgravity conditions are required in these measurements to greatly reduce static pressure variations across the sample under study, thus providing a more homogeneous sample in which to study dynamic critical phenomena.

Task Description:

Earth's gravity stabilizes the He-I/He-II interface in ground-based research. However, in microgravity only very precise heat flux control may be used to stabilize this interface. Hence, two major technical advances are required to stabilize and accurately measure the thermal profile near the interface in microgravity. First, thermometers must be developed with adequate temperature resolution to measure these very small thermal gradients without creating perturbations with its self-absorbed heat from cosmic radiation. Secondly, the experimental cell and support structure must provide an extremely high level of thermal isolation between thermometry probes along the column of helium, and must possess adequate stray heat control from other stages within the cryoprobe. In order to obtain thermal gradient information close to the interface, and hence very close to criticality, spatial resolution of the thermometry probes along the helium column must be no worse than $12\text{ }\mu\text{m}$. We intend to make measurements of the interface thermal profile using $5\text{ nW/cm}^2 < Q < 70\text{ nW/cm}^2$ on Earth orbit.

Task Significance:

The improvements to the HRT's developed for the CHeX mission will also be applied to the DYNAMX HRT's. The composite construction of the conductivity cell will reduce its mass substantially from those of the LPE and CHeX sample cells, thereby reducing the degradation of the measurement resolution in orbit caused by ionizing radiation.

Progress During FY 1996:

We have developed a cryostat for use at the University of New Mexico which contains a novel caged cell design to carefully control stray heat, and a set of four CHeX-like HRTs with a demonstrated resolution of $2 \times 10^{-10}\text{ K}$ near 2.177 K and a drift rate of a few tens of femptokelvins (femptokelvins = 10^{-15} Kelvins) per second. By heating the helium thermal conductivity cell from above, we have achieved a state of self-organized criticality, which was predicted theoretically in the mid-1980s. Here the normal fluid phase of helium within the cell self-organizes to a constant thermal conductivity such that the thermal gradient induced by the applied heat flux exactly equals the gradient in the superfluid transition temperature induced by Earth's gravity, leaving the entire height of normal fluid at a constant effective reduced temperature, and hence at a constant distance from criticality. This state has been used to observe the stability of the interface in an experimental configuration which more closely resembles microgravity conditions than does the conventional heat-from-below configuration on Earth. We observe that the interface between this SOC state of He-I and the He-II phase is stable. In order to investigate the stability and control of the interface in true microgravity conditions, Prof. Peter Weichman and his students at Caltech have performed a detailed theoretical stability analysis based on 'Model F' of Halperin and Hohenberg for the critical

dynamics near the superfluid transition. They find that the interface should remain stable under microgravity conditions in a heat flux. These experimental and theoretical results in support of DYNAMX are now being prepared for publication in refereed journals.

In preparation for space flight, we have studied the level and effects of cosmic radiation heating on the DYNAMX apparatus. This study has mandated the design of a HRT with less than 10 picowatts total power absorption from cosmic radiation, and a careful mass balance throughout the caged cell design to assure adequate control of stray heat. Other aspects of the flight apparatus, such as vapor bubble pressure regulation, have also been studied. A vespel thermal conductivity cell has been developed and used in the cryostat described above. A similar cell has survived a shake to launch specifications.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 3

TASK INITIATION: 1/93 EXPIRATION: 12/01

PROJECT IDENTIFICATION: 963-24-04-04

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Adriaans, M.J., Moeur, W.A., Boyd, S.T.P., Strayer, D.M., and Duncan, R.V. Cryogenic design of the liquid helium experiment 'Critical Dynamics in Microgravity'. Cryogenics, vol. 36, 787 (1996).

Duncan, R., Boyd, S., Moeur, W., Robinson, S., Akau, R., and Gianoulakis, S. Critical Dynamics in Microgravity. International Journal of Thermophysics, vol. 17, 631 (1996).

Proceedings

Liu, F. C., Duncan, R., Israelsson, U., Chui, T., Hensinger, D., Nash, A., Adriaans, M., and Moeur, W. "Effect of gravity on thermal conductivity measurement of 4He near Tl." Proceedings of the 21st International Conference on Low Temperature Physics LT-21 (Prague), Czechoslovak Journal of Physics, vol. 46, Supplement S1, 87 (1996).

Nash, A.E., Mukharsky, Y.M., Aaron, K.M., and Paine, C.G. "Development of structural and thermal elements for Critical Dynamics in Microgravity Experiment." Proceedings of the 35th Aerospace Sciences Meeting, Reno, NV (1996).

Satellite Test of the Equivalence Principle (STEP)

PRINCIPAL INVESTIGATOR: Prof. C. W. F. Everitt

Stanford University

CO-INVESTIGATORS:

Worden, P.

Stanford University

Task Objective:

The objective of the Satellite Test of the Equivalence Principle (STEP) experiment is to investigate the foundation of gravitational theory, the equivalence of inertial and gravitational mass.

Task Description:

The mission, now called MiniSTEP, is a NASA-led experiment with possible collaboration with the European Space Agency. The MiniSTEP mission is a descoped QuickSTEP mission with the essential Equivalence Principle science intact. The overall cost has been reduced from approximately \$600 million (for the M2 STEP, with 5 co-experiments) to ~\$50 million for MiniSTEP alone.

Task Significance:

The STEP experiment may be thought of as a modern version of the experiment attributed to Galileo of dropping two weights from the Leaning Tower of Pisa. Any difference in the ratio of gravitational to inertial mass causes a corresponding difference in the rate of fall. The detection of a difference would substantially alter present theories of relativity and gravitation.

Progress During FY 1996:

- (1) We have made minor improvements to the Flux Microscope. Samples prepared at JPL were tested and shown to be inadequate for our purposes. We are currently searching for a new supplier of EuSe samples. We are still waiting for usable Nb/EuSe samples.
- (2) The SQUID Position Sensor test bed has undergone its third major revision. The position sensing will use a commercial SQUID sensor in conjunction with GP-B SQUID electronics. Quartz flats are now being used to support niobium thin film pick-up coils. The quartz flats allow for better pick-up coil/test mass alignment. The manufacture of the pick-up coils is now all done in-house at Stanford. Designs for a differential sensor have begun.
- (3) We made further improvements to the Exposure System which can now expose niobium circuits on cylinders. A new cylinder positioner aligns the cylinders within 1 micron. This system is reproducible to better than 1 micron and has a resolution of about 3 microns. We developed special software to drive this system since commercial software was not up to the job. We have made measurements of the systematic errors and determined that improved motors and encoders will be needed, as well as a longer horizontal stage.
- (4) The Electrostatic Positioning System (EPS) is currently capable of making position measurements in six degrees of freedom. The components for the voltage control have been acquired but not assembled. The EPS has been shown to detect position at the submicron level. Verification at the 1nm level requires a test bed that we are in the process of developing. A modified version of this test rig will also be used with the tipper table. The mock test mass (aluminum) has been manufactured. The electrode housing has been designed and will be manufactured in-house at Stanford. We have also machined a mock test mass cube made of silica aerogel. We plan to adopt a dc suspension system (taking advantage of the work in progress on GP-B). We are currently using the ac suspension system developed for the GP-B gyroscopes to suspend our mock test mass.
- (5) We have assembled the major components of the tipper table and are working to operate it with a wirewound superconducting bearing until thin film bearings and the electrostatic suspension are available. This allows us to develop the basic control law and method while waiting for the electrostatic development, since the wire bearing can be operated in one g. Soon we expect to be able to use a GP-B suspension and aluminum mock test mass in this apparatus with a good chance of upgrading to an aerogel test mass.

(6) Last year we built a vacuum probe for helium storage dewars, and constructed a simple magnetometer for flux motion measurements, using a Quantum Design DC SQUID. This has been extremely successful and we have extended the range of flux motion measurements significantly. The vacuum probe is so useful that we are building a second one to study superconducting-superconducting junctions and heat switches.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	3	PhD Degrees:	1

TASK INITIATION: 10/84 EXPIRATION: 9/95

PROJECT IDENTIFICATION: 962-24-07-10

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Everitt, C.W.F. "Update on MiniSTEP." International Workshop of the Fundamental Physics Advisory Group, Headquarters of the European Space Agency, Paris, France, April, 1996.

Everitt, C.W.F. "Satellite Test of the Equivalence Principle (STEP)." 9th Russian Gravitational Conference, Novgorod, Russia, June, 1996.

Everitt, C.W.F. "The NASA/ESA miniSTEP Experiment." COSPAR, Birmingham, U.K., July 7, 1996.

Sapilewski, G. "Differential accelerometer testing apparatus." Symposium on Fundamental Physics in Space, London, October 1995.

Torii, R. "SQUID position sensor for the Stanford accelerometer." Symposium on Fundamental Physics in Space, London, October 1995.

Worden, P. "The MiniSTEP experiment." MiniSTEP 'New Ideas' Session, Jet Propulsion Laboratory, May 1996.

Worden, P. "The equivalence principle experiment on MiniSTEP." International Scientific Workshop, European Space Agency Headquarters, Paris, April 1996.

Worden, P. "Testing the equivalence principle in space." 1996 April Meeting of the American Physical Society, Indianapolis, May 1996.

Worden, P. "Accelerometer development at Stanford." Symposium on Fundamental Physics in Space, London, October 1995.

Critical Fluid Light Scattering Experiment - ZENO

PRINCIPAL INVESTIGATOR: Prof. Robert W. Gammon

University of Maryland

CO-INVESTIGATORS:

Shaumeyer, J.N.

University of Maryland

Task Objective:

The objective is to measure the decay rates of critical density fluctuations in a simple fluid (xenon) very near its liquid-vapor critical point using laser light scattering and photon correlation spectroscopy. Such experiments are severely limited on Earth by the presence of gravity which causes large density gradients in the sample. The goal is to measure fluctuation decay rates with 1% precision two decades closer to the critical point than is possible on Earth, with a temperature resolution of ± 3 micro-Kelvin. This will require loading the sample to 0.1% of the critical density and taking data as close as 100 micro-Kelvin to the critical temperature ($T_c = 289.72$ K). The minimum mission time of 100 hours will allow a complete range of temperature points to be covered, limited by the thermal response of the thermostat and correlation averaging times. Other technical problems have been addressed such as multiple scattering and the effect of wetting layers.

Task Description:

We have demonstrated the ability to avoid multiple scattering by using a thin sample (100 microns), a fast optical thermostat with micro-Kelvin temperature control and measurement, and accurate sample loading. Further, the important engineering tasks of mounting the experiment to maintain alignment during flight have been confirmed.

The experiment entails measurement of the scattering intensity fluctuation decay rate at two angles, 12 and 168 degrees, for each temperature and simultaneously recording the scattering intensities and sample turbidity (from the transmission). The analyzed intensity and turbidity data gives the correlation length at each temperature and locates the critical temperature.

The fluctuation decay rate data set from these measurements will provide a severe test of the generalized hydrodynamics theories of transport coefficients in the critical region. When compared to equivalent data from binary liquid critical mixtures they will test the universality of critical dynamics.

Task Significance:

Such experiments are severely limited on Earth because gravity causes a large density gradient in the fluid due to the divergence of the fluid compressibility as the critical temperature is approached. The data from this experiment will provide a test of critical phenomena theories in a temperature realm that has not been adequately tested to date, due to the limitations imposed by gravity. The data tests the current theory of crossover from asymptotic behavior near T_c to pure background behavior far from T_c . Such a crossover theory is useful for predicting thermophysical properties in supercritical fluid solvents.

Progress During FY 1996:

We successfully completed a second run of Zeno on USMP-3, STS-75, Feb. 22, 1996. The strategy of log scaled ramps was successful in avoiding the density perturbations seen on the first flight. Thus we achieved for the first time in microgravity excellent density stability as measured by the interference effect on the sample transmission. On the tenth day of we were at about 1 milliKelvin from T_c when we changed laser power from 17 micro-W to 1.7 micro-W. This caused a surprisingly large change in transmission signal which we could interpret as a very large (0.6%) change in local density. From that time on, the local density at the laser position was in monotonic drift. Post flight study indicates that this was due to a local heating from the previously measured 28 ppm absorption of the pair of window surfaces next to the sample volume probed by the laser.

We have completed the post-flight instrument checks and found no anomalies. We have very nice and stable cell fringe data so we are in a position to unfold the forward-backward scattering ratios from the effects of window reflection (with interference). Once this is done, the forward-backward scattering intensity ratios lead directly to a measurement of the correlation range. We then will compare our decay rate measurements with the theoretical

predictions for scaling with reduced wavevector. The focus of the study shifts from saying how close we got to T_c to saying how large the correlation range had become. We will return to the first flight's data with this analysis also.

The flight apparatus has been turned over to LERC where it is assembled for further ground operation and storage for future use. Because of the difficulty controlling the local density in microgravity, it was decided not to remove the sample cell for gas analysis.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	5	PhD Degrees:	4

TASK INITIATION: 12/88 EXPIRATION: 2/97

PROJECT IDENTIFICATION: 963-50-0C-25

NASA CONTRACT NO.: NAS3-253

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Palik, E.D., Boukari, H., and Gammon, R.W., Experimental study of the effect of surface defects on the finesse and contrast of a Fabry-Perot interferometer. *Appl. Optics*, 35, pp. 38-50 (1996).

Palik, E.D., Boukari, H., and Gammon, R.W., Experimental study of the effect of surface defects on the finesse and contrast of a Fabry-Perot interferometer. *Appl. Optics*, 35, pp. 38-50 (1996).

Zhang, K.J., Briggs, M.E., Gammon, R.W., and Sengers, J.V., Optical measurement of the Soret coefficient and the diffusion coefficient of liquid mixtures. *J. Chem. Phys.*, 104, pp. 6881-6892 (1996).

Presentations

Gammon, R.W., "Development and flight of the Zeno experiment at the University of Maryland." invited paper at the Human Exploration & Development of Space Conference, University of Maryland, November 8, 1995.

Gammon, R.W., Shaumeyer, J.N., Briggs, M.E., Boukari, H., and Gent, D.A., "Zeno: critical fluid light scattering experiment." paper #43 at the Third Microgravity Fluid Physics Conference, June 13-15, 1996.

Gammon, R.W., Shaumeyer, J.N., Briggs, M.E., Boukari, H., and Gent, D.A., "Zeno: comparison of critical fluctuation PCS on Earth and in low gravity." paper at the Photon Correlation and Scattering Topical Meeting, Optical Society of America, Capri, Italy, August 1996.

Gammon, R.W., Shaumeyer, J.N., Briggs, M.E., Boukari, H., and Gent, D.A., "Zeno: critical fluid light scattering in microgravity." invited paper at the NATO Advanced Research Workshop, Jagiellonian University, Krakow, Poland, August 1996.

Confined Helium Experiment (CHeX)

PRINCIPAL INVESTIGATOR: Prof. John A. Lipa

Stanford University

CO-INVESTIGATORS:

Chui, T.C.P.

Israelsson, U.E.

Gasparini, F.M.

Jet Propulsion Laboratory (JPL)

Jet Propulsion Laboratory (JPL)

State University of New York, Buffalo

Task Objective:

Of significant current interest in the field of condensed matter is the study of crossover behavior as a bulk system is confined more and more tightly in one or more dimensions. Crossover occurs when the effect of the boundaries is significant but not dominant. An ideal way to explore this effect is to perform measurements on films of ever decreasing thickness until the lower dimensional behavior is dominant. Unfortunately, in most cases it is not possible to vary the film thickness without totally changing the sample, making it difficult to keep track of intrinsic changes in the parameters. Also, in real systems other effects often dominate the behavior of matter at very small length scales. Near the lambda transition of helium the correlation length diverges, magnifying the effects of the confinement while simultaneously decreasing the importance of extraneous effects. This situation gives us a unique tool to look at a diverse set of conditions in a controlled way, opening a new window on the general question of finite size phenomena in condensed matter systems. For example, at 0.1C below the transition, the correlation length is on the order of a few Angstroms, whereas 10^{-9} degree below the transition the correlation length is about 0.1 mm. This means that, if we can access the inner region very close to the transition, we will have for the first time a finite size system with a truly macroscopic length scale, allowing exceptional control of the effects of boundaries. This situation appears to be absolutely unique in condensed matter systems. The Confined Helium Experiment should lead to dramatically improved tests of the theory of finite size effects.

Task Description:

We plan to measure the heat capacity of helium confined between closely spaced parallel plates and compare the results with the bulk heat capacity data obtained on the Lambda Point Experiment (LPE). The relationship between the two data sets is predicted by theories of confinement. Most of the LPE flight hardware will be reused to perform the required measurements.

Task Significance:

The Confined Helium Experiment should provide a much improved test of the theory of confinement and may provide a firm basis for its extension to other properties of confined materials.

Progress During FY 1996:

In the past year instrument testing has been completed, and the CHeX instrument was successfully integrated with the flight cryostat and electronics. The performance of the instrument has been demonstrated to be sufficient to meet all science requirements and most goals. The only goal shortfall is a current limit of 0.02% in the accuracy of the heat capacity measurements, a factor of two worse than desired. This disparity appears to be a problem with an analogue-to-digital converter calibration and is being worked. The environmental test program was completed and a number of small discrepancy items were corrected. A critical science area was susceptibility to radiated EMI (electromagnetic interference), a major problem on our previous flight experiment, the Lambda Point Experiment. The current experiment experienced no problems from EMI. All looks good for a '97 launch.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 0

PhD Students: 2

TASK INITIATION: 12/92 EXPIRATION: 12/97

PROJECT IDENTIFICATION: 963-24-04-02

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Lipa, J. A. "Critical phenomena in microgravity: past, present, and future." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13845, 8-12 (1996).

Swanson, D. R., Nissen, J. A., Qin, X., Lipa, J. A., Chui, T. C. P., Israelsson, U. E., and Gasparini, F. M. "Heat capacity of confined helium very near the lambda point." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13845, 13-16 (1996).

A New Test of Critical-Point Universality by Measuring the Superfluid Density Near the Lambda Line of Helium

PRINCIPAL INVESTIGATOR: Prof. John A. Lipa

Stanford University

CO-INVESTIGATORS:

Dohm, V.

Israelsson, U.E.

DiPirro, M.J.

Technische Hochschule Aachen
Jet Propulsion Laboratory (JPL)
Goddard Space Flight Center (GSFC)

Task Objective:

The objectives of the first year's activities were to optimize the design of the apparatus based on the experience gained from laboratory work to date and existing flight programs, begin work on the Science Requirements Document, and set up a laboratory model of the experiment.

Task Description:

We planned to study the optimization of the apparatus based on experience gained from laboratory work to date and existing flight programs. The output of this effort will be a set of science guidelines and proposed techniques to optimize the return from the flight experiment. This output will be in the form of a Science Requirements Document and a set of related engineering recommendations. Careful consideration will have to be given to the mission time and orbit constraints, and we plan some effort to ensure that the mission time line has the maximum degree of flexibility.

Part of the study will be devoted to an in-depth analysis of the theoretical position with respect to the proposed measurements, along with simulations of the expected data and its analysis to derive the tests of interest. In parallel with this activity an improved theoretical analysis of the Wegner corrections and other issues will be commenced by V. Dohm's group.

We also planned to develop a specially configured resonator designed for use as a simulation of the flight configuration, and to begin testing it in a prototype instrument. This task will involve the construction of a prototype probe of the type expected to be used on the mission. This will be similar to that used for the LPE and CHEX programs. The purpose of this work will be to get a better idea of the technical challenges in the new experiment before significant effort is put into a flight resonator, and to give the science team as much experience as possible with the phenomena expected in flight.

Task Significance:

The output from the task should lay the scientific groundwork for the flight experiment.

Progress During FY 1996:

This task started very late in FY 1996.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION:

RESPONSIBLE CENTER: JPL

In Situ Monitoring of Crystal Growth Using MEPHISTO

PRINCIPAL INVESTIGATOR: Dr. Reza Abbaschian

University of Florida

CO-INVESTIGATORS:

Coriell, S.R.

National Institute of Standards and Technology (NIST)

Allen, D.

University of Florida

deGroh III, H.C.

NASA Lewis Research Center (LeRC)

De Vahl Davis, G.

University of New South Wales, Australia

Task Objective:

The objective is to determine the morphological stability of solid/liquid interfaces and resulting macro and micro segregation patterns, and to determine the attachment kinetics at the freezing interface deduced via measurements of the growth-rate/interface-supercooling relationship.

Task Description:

To investigate the solidification behavior and stability of solid/liquid interfaces during the growth of pure Bi (a facet forming material), and Bi alloyed with small amounts of Sn, in 1-g and μ g. The experiments are designed to use the fourth flight in space of the solidification furnace known as MEPHISTO, scheduled for launch October, 1997.

The experiments make use of the Seebeck technique to measure the interface temperature in-situ and non-invasively during crystal growth in both the ground-based and flight experiments. Both 1-g and μ g experiments make use of the measured resistance change across the sample to determine interfacial velocity and Peltier pulsing for demarcation of the interface shape. Extensive analytic and numerical modeling of the solidification process is also being done.

Task Significance:

The experiments will be performed to gain a detailed understanding of the role of gravity driven convection during the solidification of faceted materials. Two fundamental and interrelated aspects of the liquid to solid transformation will be investigated: (a) Morphological stability of the solid/liquid (s/l) interfaces and the resulting macro- and micro-segregation patterns and (b) atomic attachment kinetics at the freezing interface, deduced via measurement of the growth rate-interface supercooling relationship(s)

Initial ground-based experiments were carried out using high purity Bi and dilute Bi-Sn alloys. Bi-Sn alloys were chosen to complement the experiments conducted by CENG/CNES on the first flight of MEPHISTO (MEPHISTO-1). On this first flight, dilute, non-faceted Sn-Bi alloys were used. The most current research program (i.e., the fourth flight of MEPHISTO, or MEPHISTO-4) will use strongly faceted Bi- 1.0 at % Sn alloys. In this manner, the results of the earlier flights are being used to compare and contrast various fundamental aspects of solidification without and with a strong influence of atomic attachment kinetics, respectively, in the presence (ground-based studies) and near-absence (μ -g studies) of gravity induced convection. It is expected that this comprehensive investigation approach will significantly further our understanding of key crystal growth parameters.

We expect to use these data to test and improve current solidification theories. In particular, the interplay between morphological stability and interface kinetics is not well understood. The microgravity experiments will yield an integrated database involving interface velocity/interface shape/interface supercooling. Such data are important from both practical and theoretical standpoints. For example, a knowledge of the transition from a faceted to a rough interface (from the Seebeck data) and the interface shape (from solute-dump-demarcated interfaces) under identical growth conditions has important applications in practical crystal growth situations. The information can be used to understand the correlation between defect generation and solute banding. In addition, because the information has been obtained in diffusion dominated conditions without the overriding effects of gravity-induced thermo-solutal convection, meaningful tests (and appropriate refinements) of the current crystal growth theories can be made.

Progress During FY 1996:

A One-Year Post Flight Report detailing the results to that date on the second flight of MEPHISTO was completed and submitted to NASA. MEPHISTO-2 provided the first unambiguous demonstration of the unexpectedly large influence anisotropies in interfacial kinetics and surface energies play in controlling the morphological stability of faceted alloys.

NASA's Microgravity Science and Applications Division (MSAD) accepted the request for reflight of this research on MEPHISTO-4 after peer review through the Hardware Reflight Review (MHRR) process.

A schedule has been engineered in preparation for the Space Flight of MEPHISTO-4, including preparation of samples, ground testing and research, testing in-flight models in France, and analytic and numerical modeling. All teams are on schedule for the launch.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 4
PhD Students: 0

TASK INITIATION: 1/90 EXPIRATION: 9/95

PROJECT IDENTIFICATION: 963-25-05-04

NASA CONTRACT No.: NAG3-109

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Coriell, S.R., Murray, B.T., Chernov, A.A., and McFadden, G.B. Effects of shear flow and anisotropic kinetics on the morphological stability of a binary alloy. *Metalurgical and materials Transactions*, vol. 27A, 687-694 (1996).

Proceedings

Abbaschian, R. Gokhale, A.B., and Allen, D.B. "A study of directional solidification of faceted Bi-Sn alloys in microgravity." *Solidification Science and Processing*, ed. Ohnaka, I. and Stefanescu, D.M., TMS, pp. 73-84, 1996.

Presentations

Abbaschian, R. and Coriell, S.R. "In situ monitoring of crystal growth using MEPHISTO." *NASA Microgravity Materials Science Conference*, NASA # LP 3342, pp. 71-76, October, 1996.

Coupled Growth in Hypermonotectics

PRINCIPAL INVESTIGATOR: Dr. J. B. Andrews

University of Alabama, Birmingham

CO-INVESTIGATORS:

Coriell, S.

National Institute of Standards and Technology (NIST)

Task Objective:

Coupled Growth in Hypermonotectics (main task)

The objective of this investigation is to gain an improved understanding of solidification processes in immiscible alloy systems. A portion of this study involves experimentation which will permit steady-state coupled growth of hypermonotectic composition samples to produce aligned microstructures. A parallel effort is underway to develop a model for the coupled growth process in monotectic systems. This analysis starts with the basic equations for diffusion controlled growth and avoids many of the simplifying assumptions often utilized in similar analyses. Once results are obtained from experimentation, they will be compared to predictions from the model and utilized to improve the model. In order to permit steady-state coupled growth in hypermonotectic composition samples, experimentation must be carried out under low-gravity conditions.

Wetting Characteristics of Immiscibles (subtask)

The objective of this glovebox investigation is to determine the influence of alloy/ampoule wetting characteristics on the segregation of immiscible liquids during microgravity processing. The most common segregation mechanism in immiscible alloys is gravity-driven segregation due to the density differences between the immiscible liquids. However, segregation is observed in many cases even when immiscible alloys are processed under microgravity conditions. While all of the operative segregation mechanisms are not completely understood, one of the most important appears to be the wetting characteristics between the immiscible phases and the ampoule. This investigation will focus on understanding the details of segregation driven by the wetting characteristics of the alloy and ampoule during low-gravity processing.

Task Description:

Coupled Growth in Hypermonotectics (main task)

This project includes the major research tasks of microgravity and ground-based experimentation, ampoule development, and theoretical modeling. Ampoule development first involved the selection of an appropriate ampoule material based on wetting characteristics and resistance to attack by the molten aluminum-indium alloy. This first step was then followed by design of an appropriate ampoule assembly to control thermal end effects and to eliminate free surfaces during microgravity experimentation. The modeling segment involves stability calculations to determine the gravity level limits and thermal gradient requirements for proper processing as well as modeling of the solidification process. In addition, the project has been concerned with the evaluation of current flight hardware for use in experimentation and with input into the development of new hardware. Experimentation requires directional solidification of immiscible aluminum-indium alloys under low-gravity conditions in order to avoid convective instability and promote steady-state coupled growth. The first set of microgravity experiments was carried out during the Life and Microgravity Spacelab mission during the summer of 1996.

Wetting Characteristics of Immiscibles (subtask)

In this glovebox investigation transparent metal analog samples will be utilized in order to study the influence of alloy/ampoule wetting characteristics on the phase separation and segregation process. The succinonitrile-glycerine alloy system will be utilized along with a glass/teflon sample cell. The succinonitrile-glycerine sample will be heated until it melts and mixes and then will be viewed through a microscope as it cools and solidifies in order to observe any wetting phenomena. The observations will be recorded on video tape for subsequent study and analysis. A range of alloy compositions will be utilized which will permit varying the relative volume fractions of the two phases and changing from a perfectly wetting to a non-wetting minor liquid phase.

Task Significance:

Coupled Growth in Hypermonotectics (main task)

The significance of this project lies primarily in the scientific gains to be made in truly understanding the coupled

growth process in immiscible alloys. Many alloys in immiscible systems have great promise for potential applications in areas which include superconductors, magnetic materials, catalysts, and electrical contacts. However, there are many details of the solidification process that are poorly understood for immiscible alloys because these details are masked by gravity-driven phenomena. This project is aimed at using the unique environment available in space to improve this understanding in order to make possible the production of new materials using specialized processing techniques.

Wetting Characteristics of Immiscibles (subtask)

Immiscible alloys show promise for use in many applications. For example, some immiscible alloys may be used to produce filters which can remove micron sized particles for medical applications. Other alloys are expected to exhibit superconducting characteristics or have unusual magnetic properties. However, in order to obtain these characteristics it is necessary to prevent the segregation problems that hinder the ability to form desired microstructures in immiscible alloys. The results of this study will clearly demonstrate the influence of one important factor, wetting behavior, on the segregation of phases in immiscible systems.

Progress During FY 1996:

Coupled Growth in Hypermonotectics (Main Task)

A great deal of work was completed on this project during FY96. First, several prototype aluminum nitride ampoule assemblies were designed and tested using the engineering model of the Advanced Gradient Heating Facility (AGHF) at the French Space Agency (CNES) in Toulouse, France. Additional testing was carried out at the Marshall Space Flight Center using the breadboard model of the High Gradient Furnace with Quench (HGFQ). Information gained from these experiments was used to select a final ampoule assembly design for flight. Qualification ampoules were delivered and tested for over temperature performance and the ability to withstand launch vibrational loads. Flight ampoules were delivered to CNES early in 1996, and were integrated for flight.

Three flight samples were processed aboard the Life and Microgravity Spacelab during the seventeen day mission from June 20 to July 7, 1996. All samples were to be processed under essentially identical conditions. However, some last minute difficulties during the flight made it necessary to process the first of the three samples under a different attitude than the others. In addition, a still unexplained malfunction resulted in the loss of data from the second sample shortly after the start of directional solidification. This data loss will obviously impact the ability to make sound scientific conclusions from this sample. However, microstructural analysis will still be possible and will yield new information on the ability to obtain desirable microstructures in hypermonotectic alloys.

Major advances have been made in the modeling area. Calculations have been made to emulate the flow patterns and velocities anticipated at different gravity levels while processing. These two and three dimensional analyses have permitted determination of the sensitivity of the experiment to residual acceleration levels and orientations with respect to the ampoule axis.

The solidification model, which starts with the basic equations for diffusion controlled growth, has been further refined. This model has already shown that some of the assumptions which were previously thought to be valid placed major restrictions on the phase equilibria conditions. The model has now been expanded to permit determination of the influence of a high diffusivity in one of the product phases during coupled growth. This addition is significant because one of the product phases is a liquid. The results indicate that diffusion in one of the phases has a surprisingly small impact on the resulting microstructure. Further analysis has been carried out to predict the influence of surface tension driven flows at liquid-liquid interfaces at the solidification front. Again the results indicate that these flows will have a relatively minor impact on the resulting microstructure. Work is continuing in this area.

Wetting Characteristics of Immiscibles (Subtask)

This glovebox investigation has developed essentially from scratch during the past year. The project involves processing succinonitrile-glycerine samples of various compositions in a microgravity environment in order to determine the influence of wetting characteristics on resulting microstructures. During the past year flight equipment to heat and homogenize the samples has been designed and construction has begun on a flight trainer. Cell design and construction has been finalized and a specialized reusable sample holder assembly has been designed. Evaluation of the trainer and cell holders is scheduled to start early in FY97.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	0
MS Students:	2	MS Degrees:	1
PhD Students:	2	PhD Degrees:	0

TASK INITIATION: 1/93 EXPIRATION: 1/98

PROJECT IDENTIFICATION: 963-25-08-09

NASA CONTRACT NO.: NAG8-397

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Andrews, J.B., Hayes, L.J., Arikawa, Y., and Coriell, S.R. Microgravity Processing of Immiscible Aluminum-Indium Alloys. *Advances in Space Research*, (accepted for publication).

Andrews, J.B., Hayes, L.J., Arikawa, Y., O'Dell, J.S., and Cheney, A.B. Microgravity Solidification of Immiscible Alloys. *Materials Science Forum* (Transtec Publications, Roosz and Rettenmayr, eds.), 50-66 (1996).

Hayes, L.J., and Andrews, J.B. The Effect of Convective Instability on Coupled Growth of Hypermonotectic Alloys. *Materials Science Forum* (V215-216, Transtec Publications, Roosz and Rettenmayr, eds.), 283-290 (1996).

Proceedings

Andrews, J.B., Hayes, L.J., Arikawa, Y., O'Dell, S., and Cheney, A. "Coupled Growth in Immiscible Alloys." *Proceedings ("Space Processing of Materials") of the Annual Meeting of the International Society for Optical Engineering-SPIE, V2809* N. Ramachandran, ed., 12-22 (1996).

Andrews, J.B. "Coupled Growth in Hypermonotectics." *Extended Abstract, Microgravity Materials Science Conference, Report Summaries Volume*, pp 30-31, 1996.

Andrews, J.B., O'Dell, J.S., Cheney, A.B., Arikawa, Y., and Hayes, L.J. "Ampoule Design and Testing for Microgravity Experimentation on Coupled Growth in Hypermonotectics." *Proceedings of the 8th International Conference on Experimental Methods for Microgravity Materials Science*, a publication of the Minerals, Metals and Materials Society, R.S. Schiffman, ed., 1996.

Arikawa, Y., Andrews, J.B., Coriell, S.R., and Mitchell, W.F. "Numerical Simulation of Directional Solidification of Hypermonotectic Alloys." *Proceedings of the 8th International Conference on Experimental Methods for Microgravity Materials Science*, a publication of the Minerals, Metals and Materials Society, R.S. Schiffman, ed., 1996.

Presentations

Andrews, J.B. "Coupled Growth in Hypermonotectics." *Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.*

Andrews, J.B., Hayes, L.J., Arikawa, Y., and Coriell, S.R. "Microgravity Processing of Immiscible Aluminum-Indium Alloys." *31st Scientific Assembly of COSPAR, Birmingham, England, July 14-21, 1996.*

Andrews, J.B., Hayes, L.J., Arikawa, Y., O'Dell, J.S., and Cheney, A. "Coupled Growth in Immiscible Alloys." *Annual Meeting of the International Society for Optical Engineering SPIE, Denver, Colorado, August 4-5, 1996.*

Andrews, J.B., O'Dell, J.S., Cheney, A.B., Arikawa, Y., and Hayes, L.J. "Ampoule Design and Testing for Microgravity Experimentation on Coupled Growth in Hypermonotectics." *TMS Annual Meeting, Anaheim, California, February 5-8, 1996.*

Arikawa, Y., Andrews, J.B., Coriell, S.R., and Mitchell, W.F. "Numerical Simulation of Directional Solidification of Hypermonotectic Alloys." *TMS Annual Meeting, Anaheim, California, February 5-8, 1996.*

Hayes, L.J., and Andrews, J.B. "Convection in Hypermonotectic Alloys." *TMS Annual Meeting, Anaheim, California, February 5-8, 1996.*

Hayes, L.J., and Andrews, J.B. "Convective Instability in Directionally Solidified Hypermonotectic Alloys (poster presentation)." *31st Scientific Assembly of COSPAR, Birmingham, England, July 14-21, 1996.*

Fundamental Aspects of Vapor Deposition and Etching under Diffusion Controlled Transport Conditions

PRINCIPAL INVESTIGATOR: Dr. Klaus J. Bachmann

North Carolina State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The program on Fundamental Aspects of Vapor Deposition and Etching under Diffusion-Controlled Transport Conditions has the following objectives:

- (i) The development of a prototype fused silica reactor and steel second confinement shell for studies of chemical vapor deposition processes at elevated pressure and reduced gravity. The motivation for the latter condition is that dominance of forced flow conditions ($Gr \ll Re^2$) requires for ground-based experimentation high linear flow velocities, that is, Reynolds numbers close to turbulent flow, which must be avoided to simplify data analysis.
- (ii) The program aims at establishing remote real-time process monitoring and control so that the relevant experimental data are transmitted to a team of ground-based observers while the experiment progresses. For methods of real-time process monitoring, we envision a combination of p-polarized reflectance, mass spectrometric sampling, and laser light scattering.

Task Description:

The task for FY96 was to design the fused silica reactor and second confinement shell, which has been completed. A prototype fused silica reactor has been built and is now under evaluation, using thermal imaging to gather information on temperature distributions for a set of operating conditions. Also, we have advanced our theoretical understanding of p-polarized reflectance spectroscopy (PRS) by an evaluation of the precision of molecular layer growth monitoring by PRS. Furthermore, we have worked out the relationship between the measured reflectance signal and the activities of reactants and products in the surface reaction layer that is attached to the substrate. A set of drawings of the source vapor switching manifolds has been submitted to our collaborators at George C. Marshall Space Flight Center for evaluation. Future work will focus onto completing the construction and testing of the reactor/confinement shell assembly, the evaluation of real-time optical process monitoring at elevated vapor pressure, the integration of mass spectrometric sampling of product generation in relation to reactant injection, and the evaluation of $Ga_{1-x}In_xP$ heteroepitaxy on GaAs substrates. This work includes software development for process monitoring and control.

Task Significance:

The significance of the reactor design is that it addresses the problems of optimization of flow conditions, containment of high pressure gases and real-time monitoring of the deposition kinetics, which is not the case for any currently available commercial OMCVD reactor. The relationship between the activities of reactants and products in the surface reaction layer (SRL) - attached to the surface of the growing film - to the dielectric function ϵ_{SRL} , and thereby to the measured reflectance finestructure, must be known to understand the kinetics of rate limiting steps in the chemical reactions that feed heteroepitaxial growth processes. Real-time monitoring of the composition of the SRL is essential for optimum process control that preferably should be based on sensing the composition of the SRL at a given time in the growth process rather than the composition and thickness of the epitaxial film. This is so because corrective actions to deviations of the latter cannot repair the already established errors in the evolution of the heteroepitaxial stack. A patent concerning PRS (U.S. Patent No. 5,552,327, invention predating the funded program) was granted on September 3, 1996 to the PI, Ms. Amy Miller, and Prof. Nikolaus Dietz. We believe that the method will have applications beyond the specific task outlined above, which will however affect in a positive way our evaluation of possible avenues for commercialization.

Progress During FY 1996:

The reactor design envisioned for the experiments in space has been finalized. It employs an innermost reactor made from fused silica into which pulses of the process gases are injected (horizontally under ground-based conditions). A stainless steel second confinement enclosure is presently being built in our in-house machine shop. All electrical services for heating and temperature monitoring, and all cooling water are brought into this shell through the bottom plate. Two entrance and two exit ports are provided in the design for implementation of p-polarized reflectance spectroscopy (PRS) at two wavelengths with lasers and detectors mounted outside the second confinement shell. Also, two probes are provided for sampling the up- and down-stream composition of the vapor stream for real-time monitoring of source vapor injection and product formation. The design of the source vapor switching panel allows for saturation of the carrier gas by the source vapor at low pressure, thus retaining high diffusivity. Pulsed operation of the source vapor supply at high total pressure is made possible by periodically filling evacuated reservoirs, one for each source vapor, with metered amounts of the low pressure carrier gas + source vapor mixture, and pushing the contents of the reservoirs sequentially by plugs of high pressure carrier gas into the reactor. The total system lay-out for our ground-based research aims at five organometallic sources and three process gases.

We have used an existing system for pulsed chemical beam epitaxy to gain initial insights into the kinetics of epitaxial crystal growth of $Ga_xIn_{1-x}P$ on GaAs and Si(100). Under conditions of pulsed source vapor supply the PRS intensity vs. time signal can be separated into (i) a slow oscillations due to interference of the partial waves reflected from the top and bottom interfaces of the growing epitaxial film, and (ii) a finestructure oscillation having same periodicity as the source vapor injection cycle. The finestructure is associated with the build-up of a surface reaction layer (SRL), in which chemical relationship progress that drive the epitaxial crystal growth process. Starting from the Fresnel eqns. for the four layer stack ambient-SRL-epilayer-substrate, we have evaluated the precision and accuracy of monitoring molecular layer growth, which is 3-5% depending on the time allowed for averaging. Also, we have derived the relation between the PRS intensity and the activities of reactants and products in the SRL. Thus the link between the measured signal and the surface kinetics that drives heteroepitaxial growth has been established. Furthermore, we have begun an investigation of early stages of heteroepitaxy, using a combination of PRS, atomic probe (AP) methods, and high resolution electron microscopy (TEM). Since defect formation is closely tied to this initial stage and affects both the bulk properties and surface topography of the evolving heteroepitaxial stack, further investigations of this critical, but complex phase of heteroepitaxy, the conclusion of the reactor construction, and further development of the theoretical basis for real-time process monitoring will be the focus areas for the next year of research.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 1/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NCC8-95

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Bachmann, K.J., Dietz, N., Miller, A., Höpfner, C., Scroggs, J.S., Tran, H.T., Kepler, G., Ito, K., and Banks, H.T. "Real-time Monitoring of Chemical Vapor Deposition Processes: Effects of Pressure and Flow." 17th Int. Union of Crystallogr. Congress, Seattle, Washington, August 1996.

Bachmann, K.J., Höpfner, C., Sukidi, N., Miller, A.E., Harris, C., Aspnes, D.E., Dietz, N., Tran, H.T., Beeler, S., Ito, K., Banks, H.T., and Rossow, U. "Molecular Layer Epitaxy by Real-Time Optical Process Monitoring." ALE-4 Conference, Linz, Austria, July 1996.

Investigation of the Relationship between Undercooling and Solidification Velocity

PRINCIPAL INVESTIGATOR: Dr. Robert J. Bayuzick

Vanderbilt University

CO-INVESTIGATORS:

Hofmeister, W.H.

Vanderbilt University

Task Objective:

The solidification velocity of electromagnetically levitated pure nickel, pure titanium, nickel based alloys, and titanium based alloys will be measured as a function of undercooling. The alloys are chosen so that a range of equilibrium partition coefficients and interdiffusion coefficients will be examined. Each alloy has a relatively large solid solubility so that a range of compositions will be tested, while maintaining single phase solidification. The effects of varying values of solute concentration, equilibrium partition coefficient, and interdiffusion coefficient on the solidification velocity will be quantified.

Task Description:

The solidification velocities and sample temperatures will be measured in electromagnetically levitated samples using a ten by ten square array of photodiodes in conjunction with a data acquisition system. The output of each photodiode will be obtained simultaneously at rates ranging from 2ms per frame to 1 μ s per frame. The movement of the solidification front will be followed by monitoring the progression of the thermal field developed by recalescence. The velocity of the interface will be determined from the data, which will be collected as a succession of frames in time. After systematic measurement of the solidification velocity over the attainable range of undercoolings, the results will be examined in order to gain an understanding of the mechanisms controlling interface movement at varying undercoolings. The examination will be accompanied by the comparison of experimental data to theoretical predictions and possible improvements on existing theories.

Task Significance:

The quantification of the relationships between solidification velocity and undercooling will impact on the basic understanding of fundamental solidification phenomena. In turn, there will be an impact on practical applications through contributing to an understanding of microstructural control and development. Initial data indicates that solidification velocity does not continually increase with increasing undercooling in the high undercooling regime. Because the presently accepted solidification theories predict an increasing growth rate with undercooling, the work could dramatically alter theoretical approaches if the initial trend is substantiated. Alternatively, if the work ultimately confirms present expectations, the theory will receive a firm foundation for the first time.

Progress During FY 1996:

Each alloy, each pure material, and each processing environment involved in experiments conducted during the past year are listed in Table 1. The undercooling range over which solidification velocity measurements were conducted are given along with the melting temperature used to calculate the percent undercooling for each material.

Table 1 - The maximum and minimum undercooling attained for each alloy, pure material, and processing environment. Also shown is the melting temperature of each material used to calculate the percent undercooling.

Material	Processing Environment	Liquidus Temperature	Minimum Undercooling	Maximum Undercooling
Nickel	UHP He	1726 K	4.4 %T _M	15.5 %T _M
Nickel	He w/air leak	1726 K	5.0 %T _M	13.7 %T _M
Nickel	He-20H ₂	1726 K	4.6 %T _M	15.8 %T _M
Ni-0.6 a/o C	UHP He	1723 K	3.2 %T _M	14.1 %T _M
Ni-1.7 a/o C	UHP He	1712 K	5.6 %T _M	14.9 %T _M
Ni-2.8 a/o C	UHP He	1699 K	5.4 %T _M	13.6 %T _M
Ni-1.2 a/o Ti	UHP He	1712 K	4.1 %T _M	14.1 %T _M

The results for pure nickel in UHP He and He-20H₂ both demonstrate a similar dependence of the solidification velocity on the melt undercooling prior to solidification. Both data sets show that the solidification velocity increases with increasing undercooling up to about 10% T_M, and then at greater percent undercoolings the dependence of the solidification velocity on the undercooling is greatly reduced. However, while the data trend is the same for both sets of nickel results, the magnitudes of the solidification velocity in different processing environments is different. The Ni processed in UHP He results are systematically lower than the Ni processed in He-20H₂ over the entire undercooling range. These observations are quantified by the best fit power law relations for the different solidification regimes. At less than 10% T_M the fits for the UHP He results and the He-20H₂ results are $V=0.039\Delta T^{2.81}$ and $V=0.059\Delta T^{2.77}$ respectively. For greater undercoolings the data remain essentially constant with $V\approx 31.3$ m/s for the UHP He results and $V\approx 38.6$ m/s for the He-20H₂ results.

The nickel processed in the UHP He environment with a gas leak indicate that under "contaminated" atmospheric conditions the solidification velocity increases with a decreased dependence on the undercooling compared to the UHP He results. Additionally, within the undercooling range tested the solidification velocity does not indicate a discontinuity at any undercooling and is fit by the power law $V=0.35\Delta T^{1.53}$ over the entire data set. The power law relations describing the pure nickel data sets are summarized in Table 2.

Table 2 - Summary of the power law fits for the pure nickel processed in different gas atmospheres.

Material	Power Law	Undercooling Range
Nickel in UHP He	$V=0.039\Delta T^{2.81}$	$\Delta T < 10\% T_M$
Nickel in UHP He	$V\approx 31.3$ m/s	$\Delta T > 10\% T_M$
Nickel in He-20H ₂	$V=0.059\Delta T^{2.77}$	$\Delta T < 10\% T_M$
Nickel in He-20H ₂	$V\approx 38.6$ m/s	$\Delta T > 10\% T_M$
Ni in UHP He w/leak	$V=0.35\Delta T^{1.53}$	All ΔT

The Ni-0.6a/o C data shows that for this low solute concentration the behavior of the alloy is not greatly changed from that of the pure material. The data for this alloy is fit with the power law $V=0.071\Delta T^{2.53}$ at less than 10% T_M and has $V\approx 31.3$ m/s at undercoolings greater than 10% T_M. These relations show a very slight decrease in the solidification velocity of this alloy in comparison to the pure Ni results, while showing the same overall trend as the pure material. This indicates that the diffusion of the solute at the interface has a very limited effect on the growth rate of the alloy in comparison to the pure material at this low concentration. The Ni-1.7a/o C data indicate a large effect of the solute on the solidification velocity. These data sets display a more complicated dependence of the solidification velocity on the undercooling in that the data indicates different behavior over various undercooling ranges. At undercoolings <7.5%T_M the data shows slowly increasing solidification velocities, between 7.5%T_M and 11%T_M the solidification velocity data remains essentially constant at approximately 9.3 m/s, between 11%T_M and 13%T_M the solidification velocity increases rapidly. Beyond 13%T_M the solidification velocity tends to level off at ≈ 29.5 m/s. This varying solidification velocity behavior with increasing undercooling indicates that 1.7a/o carbon is a sufficient solute concentration to alter the mechanisms dominating the solidification process, i.e. diffusion of the solute at the interface is affecting the interface mobility. The 2.8a/o carbon data set shows a similar trend as the 1.7a/o C data but the solidification velocities are generally lower for equivalent amounts of undercooling. In comparison to the 1.7a/o C data the 2.8 a/o C data rises more slowly at undercoolings <9%T_M and between 9%T_M and 11%T_M the solidification velocity data remains essentially constant at the lower velocity of 5.5 m/s. The 2.8a/o data between 11%T_M and 12%T_M indicates a more rapid rise in the solidification velocity than the 1.7a/o C data over a smaller undercooling range. The average of the large undercooling points, > 12%T_M, is also lower and is ≈ 26.9 m/s. This comparison indicates an increasing effect of solute on the solidification velocity dependence on undercooling with increasing concentration. For each of the solidification velocity regimes described above a power law function was fit to the data. These fits are summarized in Table 3.

The effect of dilute additions of a substitutional alloying element on the solidification velocity of pure nickel was tested by an addition of titanium to nickel. The results for the alloy Ni-1.2a/o Ti are that at undercoolings of <10% T_M the solidification velocity of this alloy is fit with the power law $V=0.072\Delta T^{2.57}$. This indicates a slightly greater solidification velocity than pure nickel. At larger undercoolings, >10%T_M, the solidification velocity of the Ni-Ti

alloy indicates the a similar discontinuity as the pure nickel in the form of a drastically decreased dependence of the solidification velocity on undercooling. In this undercooling regime the solidification velocity is ≈ 26.9 m/s. This average velocity lies below the "plateau" region of the pure nickel results. The trends of the Ni-Ti data are summarized in Table 3.

Table 3 - Summary of the power law fits for pure nickel and the nickel alloys.

Material	Power Law	Undercooling Range
Nickel in UHP He	$V=0.039\Delta T^{2.81}$	$\Delta T < 10\% T_M$
Nickel in UHP He	$V \approx 31.3$ m/s	$\Delta T > 10\% T_M$
Ni-0.6 a/o C	$V=0.071\Delta T^{2.52}$	$\Delta T < 10\% T_M$
Ni-0.6 a/o C	$V \approx 31.3$ m/s	$\Delta T > 10\% T_M$
Ni-1.7 a/o C	$V=0.0008\Delta T^{4.48}$	$5\% T_M < \Delta T < 7.5\% T_M$
Ni-1.7 a/o C	$V \approx 9.3$ m/s	$7.5\% T_M < \Delta T < 11\% T_M$
Ni-1.7 a/o C	$V=5e-7\Delta T^{7.0}$	$11\% T_M < \Delta T < 13\% T_M$
Ni-1.7 a/o C	$V \approx 29.5$ m/s	$\Delta T > 13\% T_M$
Ni-2.8 a/o C	$V=0.003\Delta T^{3.41}$	$5\% T_M < \Delta T < 9\% T_M$
Ni-2.8 a/o C	$V \approx 5.5$ m/s	$9\% T_M < \Delta T < 11\% T_M$
Ni-2.8 a/o C	$V=2e-6\Delta T^{6.51}$	$11\% T_M < \Delta T < 12\% T_M$
Ni-2.8 a/o C	$V \approx 26.9$ m/s	$\Delta T > 12\% T_M$
Ni-1.2 a/o Ti	$V=0.072\Delta T^{2.57}$	$\Delta T < 10\% T_M$
Ni-1.2 a/o Ti	$V \approx 26.9$ m/s	$\Delta T > 10\% T_M$

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 1/00

PROJECT IDENTIFICATION:

NASA CONTRACT No.: NCC8-91

RESPONSIBLE CENTER: MSFC

Experiments on Nucleation in Different Flow Regimes

PRINCIPAL INVESTIGATOR: Dr. Robert J. Bayuzick

Vanderbilt University

CO-INVESTIGATORS:

Hofmeister, W.H.

Vanderbilt University

Robinson, M.

NASA Marshall Space Flight Center

Task Objective:

The primary objective of the research is to quantitatively measure the behavior of solid nucleation from the undercooled melt of pure zirconium as a function of undercooling and melt stirring. To enable comparisons with theory, a secondary objective is to measure the heat viscosity and the viscosity of undercooled liquid zirconium as a function of temperature.

Task Description:

Three ground-based processing techniques are being applied to nucleation experiments. The three ground-based processing techniques are electromagnetic levitation, electrostatic levitation, and free fall in long drop tubes. Ultimately, experiments will be done in low earth orbit on the Space Shuttle mission referred to as MSL-1, presently scheduled to launch in March 1997.

For every experimental set, approximately one hundred undercooling measurements are targeted. The number of experimental measurements is needed to properly interpret experimental results by applying statistical techniques. Primarily, differences and similarities of nucleation behavior under various conditions are assessed by null hypotheses testing of the means of distributions of nucleations as a function of temperature as well as the dispersion in distributions of nucleations as a function of temperature. Furthermore, a modification of Skripov's statistical approach to nucleation is applied to the results. The cumulative distribution function is obtained by numerically integrating the nucleation rate over temperature. The probability density function is used to obtain a measure of the preexponential factor and the exponential in the nucleation rate equation.

The flight experiments will involve deterring and analyzing the distribution of nucleations as a function of temperature under two well-controlled flow conditions. One condition will be in the laminar flow regime and the other in the turbulent flow regime. The flight experiments also involve measurements of heat capacity and viscosity as a function of undercooling. The heat capacity is determined by response of temperature of the melt to controlled inputs of power. The viscosity is measured by the dampening of shape oscillations of the melt.

Task Significance:

Solidification processing is one of the most prominent methods for the production of materials and most of these processes begin with a nucleation step. The regime of nucleation known as deep undercooling, where liquids are cooled considerably below their equilibrium freezing temperatures prior to the formation of solids, can be particularly distinctive. With deep undercooling, a unique condition for microstructural development and control exists. Therefore, a unique condition for improving and controlling the properties of materials exists. The full realization of exploiting such solidification processing requires an understanding of the fundamentals of nucleation in the unique deep undercooling regime.

Progress During FY 1996:

In a continuing effort to improve the theoretical and statistical foundation of the research project, the dependence of undercoolings on experimental parameters has been studied in more depth. Since a dependence on individual sample and on processing cycle number would reduce or even nullify the statistical significance of any comparisons between sets of undercoolings, these parameters have been studied closely. From regression analyses and analysis of variance techniques, it was concluded that there is no significant dependence of undercooling on individual sample or on cycle number.

Although a complete factorial design of processing method, purity, and size is not yet complete, subsets have been analyzed in order to obtain initial results. In a factorial design that encompasses the drop tube and the EML undercooling results for three purities and one size, the results indicate that increasing purity allows larger undercoolings to be obtained; however, there was greater variability in the EML undercoolings than in the drop tube. Another difference was that for the higher purity materials the drop tube undercoolings were smaller than the corresponding undercoolings for the EML. An experiment is planned using induction heating rather than the e-beam furnace during melting to determine the source of the mean undercooling differences.

In order to complete the full factorial design, experiments were performed in the newly constructed Electrostatic Levitator (ESL) at Space Systems/Loral (SS/L) in Palo Alto, California. Zirconium samples of three different sizes and three different purities were prepared for processing. At present, two full data sets of around 100 undercoolings and two partial data sets with approximately 20 undercoolings have been acquired. Initial results indicate that there is no significant difference in the mean undercooling between samples of differing sizes (1.5 mm diameter and 3.0 mm diameter). There was also no significant difference between the mean undercoolings for the 4N5 (99.995%) and 3N5 (99.95%) purity samples. In contrast, a difference was observed between these two purity levels in the Electromagnetic Levitator (EML) at Vanderbilt University. Although the mean undercoolings of approximately 330 K in the ESL for the 4N5 and 3N5 purity materials were the same as those observed for the 4N5 purity material in the EML, the variances were much less than in any EML distribution obtained. Further experiments are scheduled in the SS/L ESL in order to complete the purity level and size effect studies. The possible difference in undercoolings as caused by sample preparation, either arc melting or machining, will also be studied in order to determine flight sample preparations.

Throughout the experiments at SS/L, two optical pyrometers were used to measure the temperature of the sample. Pyrometer #1 had a silicon detector with a filter centered at 650 nm. Pyrometer #2 had an InGaAs detector filtered at 1300 nm. After extensive calibrations of both pyrometers, differences in the full width half maxima of the undercooling data sets obtained using the two pyrometers were attributed to differences in temperature resolution of the two pyrometers. However, the mean undercoolings were the same for the distributions. Further work is being done in order to determine the effects of temperature resolution on the results of statistical analyses.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 6/96 EXPIRATION: 5/98

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NCC8-101

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

NASA Tech Briefs

Rulison, A., Rhim, W.K., Morton, C.W., Hofmeister, W.H., and Bayuzick, R.J. Liquid to Solid Nucleation in Two Representative Grades of Commercially Available Zirconium. NASA Tech Brief, NPO-19727, (1996).

Presentations

Morton, C.W., Hofmeister, W.H., and Bayuzick, R.J. "The Statistical Analysis of Undercooling Data." Naval Research Laboratory, Washington, D.C., September 1996.

Equiaxed Dendritic Solidification Experiment (EDSE)

PRINCIPAL INVESTIGATOR: Prof. Christoph Beckermann

University of Iowa

CO-INVESTIGATORS:

Steinbach, I.
Murray, B.T.
deGroh III, H.C.ACCESS e.V. (Germany)
National Institute of Standards and Technology (NIST)
NASA Lewis Research Center (LeRC)

Task Objective:

The objectives of the research are to determine the microstructural evolution of and thermal interactions between several equiaxed crystals growing dendritically in an undercooled melt of a pure substance, and to use this benchmark data to test and develop equiaxed dendritic solidification models.

Task Description:

It is planned to perform well-controlled equiaxed dendritic solidification experiments on the scale of several crystals to provide benchmark data for the testing and refinement of present and future equiaxed microstructure evolution models, both in the pure diffusion limit as well as with convection. The research program is a combination of microgravity experiments (diffusion limit), corresponding ground-based experiments (with convection), and supporting analysis and simulation. The experiments will utilize a modified version of the Millikelvin Thermostat (MITH) and involve the growth of up to four equiaxed crystals of the transparent, pure model material SCN simultaneously towards each other. Of interest are the evolution of the dendrite morphology, the dendrite envelope, and the internal solid fraction in a multi-crystal setting, and the nature and interactions of the thermal fields around neighboring crystals. The influence of convection will be ascertained by comparing the results of the microgravity and ground-based experiments. Critical to the success of the research will be the planned micro- and meso-scale simulations of the experiments, enabling (i) the extraction of additional information about the relation between the experimental data and the physical conditions, and (ii) the development of refined or new models for both the diffusion and the convection case.

Task Significance:

The planned microgravity experiment will generate benchmark data for the testing and refinement of theories on equiaxed dendritic solidification of metals and alloys. The research will establish a more firm scientific basis for the numerical simulation of microstructure evolution in casting processes in order to optimize material properties. It extends previous microgravity experiments on the growth of a single, isolated dendrite tip (IDGE) to multiple crystals – a situation close to actual casting conditions.

Progress During FY 1996:

The project was initiated in June 1996 through a kick-off meeting at NASA Lewis Research Center. Definition of the science requirements has commenced and drafts are being prepared. A ground-based test setup for use at the University of Iowa is presently being designed and constructed in collaboration with personnel at NASA LeRC. All of the requirements for this setup have been defined. In addition, the microscopic and mesoscopic simulations of the planned experiments have been started.

STUDENTS FUNDED UNDER RESEARCH:BS Students: 1
MS Students: 2
PhD Students: 2

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NCC8-94
RESPONSIBLE CENTER: MSFC

Alloy Undercooling Experiments in Microgravity Environment

PRINCIPAL INVESTIGATOR: Dr. Merton C. Flemings

Massachusetts Institute of Technology (MIT)

CO-INVESTIGATORS:

Matson, D.M.

Massachusetts Institute of Technology (MIT)

Task Objective:

The objectives of this task are to perform solidification experiments on undercooling alloys, to compare results of ground-based and microgravity experiments, and to examine effects of microgravity on solidification behavior and microstructure characteristics.

Task Description:

We will collect thermal history, nucleation and growth history, and resulting solidification microstructures through experiments applying direct, high speed, high resolution pyrometric and cinematographic measurements during melting, undercooling and recalescence of different compositions, both on the ground and in microgravity.

Task Significance:

With experiments carried out in microgravity, it is expected to have improved specimen shape and stability and reduced convection during cooling, resulting in the possibility of higher undercooling, less microstructure alteration, reduced coarsening, and improved specimen observation in order to gain a complete understanding of the solidification kinetics of undercooled melts, including: primary dendrite tip velocities; rapid thickening of primary and secondary arms during recalescence; ripening, remelting, and solute redistribution; dendrite fragmentation and grain refinement; primary phase solidification and ripening; and eutectic solidification with concurrent primary phase ripening.

Progress During FY 1996:

The experiment pre-flight thermophysical property analyses have been completed based on ground-based experimentation. Recalescence velocity measurements and phase transformation delay times have been conducted on the flight steel alloys; nucleation stimulation testing has also been accomplished. Flight levitation coil configuration has been verified using the flight alloys during KC-135 microgravity testing. Ground-based tests on the flight sample holder and evaporation shield have been completed and the nucleation trigger fabricated and delivered for installation in the TEMPUS facility. Flight sample fabrication and laminar/turbulent convection testing has been initiated.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	1
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 10/95 **EXPIRATION:** 10/98**PROJECT IDENTIFICATION:** 963-35-12**NASA CONTRACT No.:** NAG8-971**RESPONSIBLE CENTER:** MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Lum, J.W., Matson, D.M., and Flemings, M.C. High-speed imaging and analysis of the solidification of undercooled nickel melts. *Met. Trans. B*, vol. 27B, 865 (1996).

Proceedings

Matson, D.M., Shokuhfar, A., Lum, J.W., and Flemings, M.C. "Imaging the double recalescence behavior of Fe-Cr-Ni steel alloys." *Solidification Science and Processing* (I. Ohnaka and D.M. Stefanescu, eds.), TMS Warrendale, Pennsylvania, p 19 (1996).

Measurement of the Viscosity and Surface Tension of Undercooled Melts Under Microgravity Conditions and Supporting Magnetohydrodynamic Calculations

PRINCIPAL INVESTIGATOR: Dr. Merton C. Flemings

Massachusetts Institute of Technology (MIT)

CO-INVESTIGATORS:

Trapaga, G.
Hyers, R.

Massachusetts Institute of Technology (MIT)

Massachusetts Institute of Technology (MIT)

Task Objective:

The objective of this investigation is to utilize the electromagnetic levitation unit, TEMPUS, on the MSL-1 space shuttle mission for the experimental determination of the surface tension and the viscosity of metallic melts, in both the superheated and the undercooled state, using the unique attributes of microgravity.

Task Description:

Metallic samples of 7 or 8 mm diameter will be positioned in the TEMPUS coils by electromagnetic forces and melted by induced currents. A "squeezing" force will then be applied to a stably positioned liquid sample to induce oscillations. The rate of decay of the amplitude of these oscillations will be observed in order to measure the viscosity at different temperatures, while the frequency of the oscillation modes will be used to deduce the surface tension at these temperatures. Measurements will be performed on reactive, refractory melts (Zr), high-viscosity eutectics (ZrNi, PdSi) and industrial alloys (Fe-Cr-Ni) in addition to standard materials for comparison (Au, Ni).

Our effort consists largely of a comprehensive program of mathematical modeling designed to give a detailed understanding of what can be expected from the flight experiments. To date, the main goal of the modeling work has been to develop the methodology and to perform calculations predicting the behavior of levitation-melted/electromagnetically-positioned metallic droplets under both earthbound and microgravity conditions. In particular, the details of the transition from laminar to turbulent flow are not well understood for this type of flow system and this issue represents a critical aspect in our research.

Task Significance:

The accurate determination of the thermophysical properties of liquid materials is important for fundamental and practical reasons, including verification of atomistic models of the liquid state, nucleation studies of phase transition and modeling of materials processing operations. To date, little study has been made of the thermophysical properties of undercooled melts, and a controversy exists over whether the temperature dependence of viscosity obeys an Arrhenius-type or a power-law relationship. In addition, the precise knowledge of how the surface tension varies with temperature is still largely unexplored.

Progress During FY 1996:

Editor's note: The Principal Investigator for this investigation was previously Dr. Julian Szekely, who passed away in December, 1995. Dr. Merton Flemings and Dr. Gerardo Trapaga assumed his responsibilities for the investigation.

Our ground preparation program is running in accordance with the original plan. Ground preparation for FY96 included the measurement of thermophysical properties of sample materials similar to those that will be used in the flight experiments; these properties include evaporation rates, coupling coefficients and spectral emissivities for the solid and liquid materials. We have also defined the flight parameter sets and verified them on flight-like hardware and software (TEMPUS demonstration model) during our visit to MUSC.

Preliminary experiments aimed at determining laminar to turbulent flow transitions have been conducted using PdSi, a material that will be used in the flight experiments. These experiments seem to indicate that the flow transition occurs within the range of processing conditions available in TEMPUS. Our refined magnetohydrodynamic finite element model of the flows in TEMPUS will allow these experimental results on laminar-turbulent transition to be applied to all TEMPUS flight samples. We have also developed custom image processing software for on-line analysis of video data which will be employed on-line during the flight experiments.

Additional ground-based experiments will be performed to further investigate the transition from laminar to turbulent flow to bracket the values of the Reynolds number involved and to investigate the effect of processing conditions for all the samples in TEMPUS.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 11/95 EXPIRATION: 11/98

PROJECT IDENTIFICATION: 963-80-05

NASA CONTRACT NO.: NAG8-118

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Egry, I., Jacobs, G., Schwartz, E., and Szekely, J. Surface Tension Measurements of Metallic Melts Under Microgravity. International Journal of Thermophysics, vol. 17, no. 5, 1181-1189 (1996).

Presentations

Flemings, M.C., Trapaga, G., and Hyers, R. "The Measurement of the Viscosity and Surface Tension of Undercooled Melts under Microgravity Conditions and Supporting MHD Calculations." Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.

Compound Semiconductor Growth in Low-g Environment

PRINCIPAL INVESTIGATOR: Dr. Archibald L. Fripp

NASA Langley Research Center (LaRC)

CO-INVESTIGATORS:

Rosch, W.R.

Debnam, W.J.

Narayanan, R.

National Research Council at NASA LaRC

NASA Langley Research Center (LaRC)

University of Florida

Task Objective:

The primary objective of this series of experiments is to determine what effects the low gravity environment has on convective mixing during the growth process. The properties of an array of devices made from PbSnTe are dependent on the ratio of the elemental components. Compositional uniformity in the resultant crystal is only obtained if the liquid is quiescent during growth.

Task Description:

The initial flight experiment on USMP-3 consisted of three separate crystals grown in a single, segmented ampoule. The crystals were grown in series, each in one of the three primary orientations with respect to the residual gravity vector. The growths on USMP-3 were analogous to hot on top, cold on top, and horizontal growth.

The new work will grow two sets of three crystals, again in segmented ampoules. The flight experiment will use the orientation that produced the most favorable growth on USMP-3. The variables, this time, will be ampoule translation rate, nucleation phenomena, and temperature gradient. The growth rate, which is related to the translation rate, and temperature gradient are key growth parameters under control of the experimenter. Higher growth rates produce steeper solutal gradients but less penetration of this vital diffusion zone into the convecting fluid flow. Thus, the growth rate presents a dichotomy of effects; a high growth rate produces a steeper concentration gradient while a low growth rate allows the diffusion tail to extend into the thermal convection cells.

Task Significance:

While one objective of this experiment is to grow PbSnTe and establish its fundamental growth properties, another, more important objective is to gain a better understanding of the mechanisms involved in generalized crystal growth, particularly those affected by gravity. This information will not only help produce better quality materials on Earth, but also help define future efforts of crystal growth in space and lead the way to more extensive materials science research.

Progress During FY 1996:

The USMP-3 flight experiment was completed in March 1996. The flight itself was successful; almost routine. The furnace powered up, the Shuttle changed attitude as scheduled, and the ampoule translated through the furnace when commanded to do so. The Advance Automated Directional Solidification Furnace (AADSDF) operated superbly producing the same temperature profiles in space as it had on the ground. The simplicity of the experiment ended with the basic flight operations.

The differences in space and ground experiments began to manifest as the first crystal started to form. The temperature signature of the crystal nucleation was much more subdued than observed in Earth based experiments. It was so muted that the experimenters used the telescience capability built into the AADSDF to re-melt the crystal and start over. The observation of beginning crystallization was verified, and thanks to the foresight of the project planners to provide this remote operating capability, the space experiment proceeded with the full confidence of the investigators.

The samples were retrieved from the Kennedy Space Center for post-flight analysis in April 1996. This analysis of the effects of microgravity growth is proceeding carefully and deliberately. Care must be taken for some of the analysis steps are destructive to the crystal. These crystals are valuable for they are all but irreplaceable, and all information must be extracted before proceeding to the next step.

So far only one of the three crystals has been cut and polished for measurement of its atomic distribution. The atomic distribution is the best measurement of convection in the liquid during crystal growth, and, of course, suppressing convection during growth was the primary goal of the experiment. The initial measurements show the effect of more convection than was hypothesized. However, optical and x-ray measurements show void, or large pore, formation in the crystals; the likes of which have not been observed in Earth grown crystals. Various reasons for this void formation are being considered, but having formed, existing theory supports the idea that the presence of voids will induce fluid flow through surface tension driven convection. The objective now is to design an experiment which will eliminate the void formation so that the original hypothesis of convection reduction in the microgravity environment can be tested.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 2
MS Students: 1
PhD Students: 0

TASK INITIATION: 10/78 EXPIRATION: 9/98

PROJECT IDENTIFICATION: 963-35-00-01

RESPONSIBLE CENTER: LaRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Barber, P., Fripp, A., Debnam, W., Berry, R., and Simchick, R. Growth rates and interface shapes in germanium and lead tin telluride observed in-situ, real time in vertical Bridgman furnaces. *J. Crystal Growth*, vol. 147, 83-90 (1995).

Matisak, B.P., Zhao, A.X., Narayanan, R., and Fripp, A. The microgravity environment: Its prediction, measurement, and importance to materials processing. *Journal of Crystal Growth*, accepted, (1996).

Matisak, B.P., Zhao, A.X., Narayanan, R., and Fripp, A. Experimental verification of agreement between thermal and real-time visual melt-solid interface positions in vertical Bridgman grown Germanium. *J. Crystal Growth*, vol 160, 55-58 (1996).

Rosch, W.R., Fripp, A.L., Debnam, W.J., and Pendergrass, T.K. Performance testing of a vertical Bridgman furnace using experiments and numerical modeling. *Journal of Crystal Growth*, accepted, (1996).

Presentations

Fripp, A.L., Debnam, W.J., Rosch, W.R., and Narayanan, R. "The effect of microgravity direction on the growth of PbSnTe." Presented at The Tenth American Conference on Crystal Growth, August 4-9, 1996, Vail, CO.

Matisak, B.P., Zhao, A.X., Narayanan, R., and Fripp, A. "The microgravity environment: Its prediction, measurement, and importance to materials processing." Presented at The Tenth American Conference on Crystal Growth, August 4-9, 1996, Vail, CO.

Rosch, W.R., Fripp, A.L., Debnam, W.J., and Pendergrass, T.K. "Vertical Bridgman research Part 1: Performance testing of a vertical Bridgman furnace." Presented at The Tenth American Conference on Crystal Growth, August 4-9, 1996, Vail, CO.

Rosch, W.R., Fripp, A.L., Debnam, W.J., and Pendergrass, T.K. "Vertical Bridgman research Part 2: Verification of a vertical Bridgman numerical model." Presented at The Tenth American Conference on Crystal Growth, August 4-9, 1996, Vail, CO.

Rosch, W.R., Fripp, A.L., Debnam, W.J., and Pendergrass, T.K. "Vertical Bridgman research Part 3: Extension of experimental measurements and numerical modeling." Presented at The Tenth American Conference on Crystal Growth, August 4-9, 1996, Vail, CO.

Gravitational Role in Liquid-Phase Sintering

PRINCIPAL INVESTIGATOR: Prof. Randall M. German

Pennsylvania State University

CO-INVESTIGATORS:

Iacocca, R.

Pennsylvania State University

Task Objective:

The purpose of this research is to establish the gravitational role in liquid phase sintering with respect to both the macro-scale distortion and phase separation, and the microstructural evolution over time at elevated temperatures.

Task Description:

The investigation has graduated to flight status, with 21 samples (seven compositions of tungsten-nickel-iron) subjected to liquid phase sintering treatments on STS-65 during July 1994. The experiments involved isothermal hold times of 1, 15, and 120 minutes at 1500°C in the Japanese-developed Large Isothermal Furnace on the IML-2 mission. Identical ground-based experiments have been conducted to provide the baseline for contrast with the microgravity samples, and post-flight analysis focuses on quantitative assessment of distortion and microstructural evolution. New theories of liquid phase sintering have resulted from the microgravity experiments. Consequently a new sample size and new composition will be processed as part of a upcoming flight, MSL-1, to show how the emerging models work.

Task Significance:

The microgravity experiments will establish a modeling basis for the gravitational role in a viscous flow distortion of sintered components. It will further assess the agglomeration of solid grains and possible coalescence contributions to grain growth for upgrading of current theories. These results will lead to the development of net shaped manufacturing techniques which will permit formulation of new unique alloys.

Progress During FY 1996:

"Sintering" means welding or fusing of metal or ceramic powders by heating them without melting. Frequently, it is aided by applying pressure in a special high-temperature press to squeeze the particles together. This experiment explores a different mechanism, by adding a portion of a powder that melts at a lower temperature and surrounds the powders that remain solid. This liquid then lets particles and materials move more easily, allowing the powders to more rapidly form a solid compact. Problems such as separation of the solid and liquid due to gravity (manifested by settling of the solid particles) still remain. Access to the low gravity environment of Earth orbit provides a unique opportunity to study liquid-phase sintering without separation, settling, or other gravity-induced complications. The results will increase our understanding of the process, and the new knowledge will help introduce new industrial application of liquid-phase sintering, such as automotive components, resulting in new and improved products.

In this investigation, mixed powders of tungsten, nickel, and iron are initially cold compacted under pressure in the shape desired for the final product. The compacts are then heated to just below the nickel-iron alloy melting temperature to provide handling strength, a process called "presintering." In the experiment, they are heated above 1465°C to form a liquid-solid mixture. The tungsten, with its very high melting point (3370°C), remains a solid, while the nickel and iron, with much lower melting points, become liquid. The liquid permits more rapid transport of material for faster sintering than would be possible if all the material were solid. After sintering, the microstructure of the samples (i.e., the structure when viewed under very high magnification), consists of connected tungsten grains surrounded by the solidified liquid.

This experiment flew as part of the second International Microgravity Laboratory (IML-2) mission in July 1994 aboard the Space Shuttle Columbia. The experiment was conducted in an apparatus called the Large Isothermal Furnace (LIF), which could operate at the high temperatures required. The LIF was developed by Ishikawajima-Harima Heavy Industries Co., Ltd., for the National Space Development Agency of Japan (NASDA). This project was supported by the NASA Headquarters Microgravity Science and Applications Division, and was managed by the NASA Lewis Research Center.

The test specimens for the LIF consisted of three different cartridges, each containing seven samples 10 mm in diameter by 10 mm high. One cartridge was tested at each of the three critical sintering periods identified in earlier ground-based experiments; 1, 15, and 120 minutes. In one minute, liquid penetrates along existing solid-solid boundaries. Fifteen minutes is the time needed for full densification. The 120-minute time is needed to observe grain rotation and coalescence events.

In summary, a nominal temperature of 1506°C was achieved for each of the desired test times. Free-drift of Columbia during the appropriate times was confirmed. All of the functional objectives were achieved. Analysis will begin upon return of the samples to the laboratories of the Pennsylvania State University.

October 1996 Update

Three dimensional pore and grain structures have been produced by serial sectioning and digital image reconstruction techniques. The product structures show some of the pores are actually very long, not isolated as previously assumed. Other tests are using two-dimensional measures of neck size, grain size, and pore size to determine if the current three-dimensional measures are predictable from two-dimensional microstructure.

A new model of grain growth has been derived based on the combined grain size measures from the ground-based and microgravity samples. This model incorporates the solid-liquid ratio, gravitational stress, and gravitational induced separation. The gravitational separation is a large contributor to grain growth in liquid phase sintering, more so than previously estimated. These findings, as well as new results on grain growth during heating, solubility effects on sintering densification and distortion, and a new model for the sintering rate have all been accepted for publication in reviewed journals.

Previous work by the Penn State team found that distortion in sintering was largely the combination of gravity and viscous flow. However, no surface tractions were included in the earlier work. Consequently, a new finite element model has been created for surface traction and gravity combinations. The results have successfully explained differences in compact shapes between microgravity and ground experiments. The microgravity compacts tend toward a spherical shape while the ground samples formed a rounded cylindrical shape. As the solid volume fraction increases, the percolation limit is exceeded and structural rigidity causes the two shapes to converge. This shows there is no gravity role in shape distortion with high solid contents. A quantitative microscopy effort is determining the connectivity and contiguity associated with microstructures that do not distort during sintering. On the basis of the new link between microstructure and compact distortion, new compositions have been formed that resist distortion during sintering with up to 80 vol. % liquid phase.

Grain growth data is being compared between the experiments performed in the two gravitational environments. The models that exist show a poor basis for explaining the observed differences in coarsening rates. The next few months will be crucial to determining the evolving microstructure, because of critical new fundamental to explaining critical events in sintering, grain growth, and distortion.

Finally, in explaining the sintering results a missing parameter is the viscosity of the solid-liquid mixture during sintering. Current calculations show values several times larger than previously suspected. New experiments are planned to determine viscosity as a function of time during sintering.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	1
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 10/94 EXPIRATION: 10/96

PROJECT IDENTIFICATION: 963-25-05-05

NASA CONTRACT No.: NAG3-128

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Bose, A., and German, R.M., Developments in the sintering of Tungsten heavy alloys. Sintering Technology, R.M. German, G.L. Messing and R.G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 269-276 (1996).

- German, R.M., Grain agglomeration in solid-liquid mixtures under microgravity conditions. *Metallurgical and Materials Transactions*, vol. 26B, pp. 649-651 (October 1995).
- German, R.M., Grain agglomeration in solid-liquid mixtures under microgravity conditions. *Metallurgical and Materials Transactions*, vol. 26B, pp. 649-651 (October 1995).
- German, R.M., The microstructures of liquid phase sintered materials. *Sintering Technology*, R.M. German, G.L. Messing and R.G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 213-220 (1996).
- German, R.M. and Liu, Y., Grain agglomeration in liquid phase sintering. *Journal of Materials Synthesis and Processing*, vol. 4, pp. 23-34 (1996).
- German, R.M. and Liu, Y., Grain agglomeration in liquid phase sintering. *Journal of Materials Synthesis and Processing*, vol. 4, pp. 23-34 (1996).
- German, R.M., Liu, Y., and Griffo, A., Gravitational effects on grain coarsening during liquid phase sintering. *Metallurgical and Materials Transactions*, (1996).
- German, R.M., Liu, Y., and Griffo, A., Gravitational effects on grain coarsening during liquid phase sintering. *Metallurgical and Materials Transactions*, (1996).
- Heaney, D.F., German, R.M. and Ahn, I.S., The gravitational effects on low solid-volume fraction liquid-phase sintering. *Journal of Materials Science*, vol. 30, pp. 5808-5812 (October 1995).
- Heaney, D.F., German, R.M., and Ahn, I.S., The gravitational effects on low solid- volume fraction liquid-phase sintering. *Journal of Materials Science*, vol. 30, pp. 5808-5812 (October 1995).
- Johnson, J.L., and German, R.M., Theoretical modeling of densification during activated solid-state sintering. *Metallurgical and Materials Transactions*, vol. 27A, pp. 441- 450 (1996).
- Johnson, J.L., and German, R.M., Solid state contributions to densification during liquid phase sintering. *Metallurgical and Materials Transactions*, (1996).
- Johnson, J.L., and German, R.M., Theoretical modeling of densification during activated solid-state sintering. *Metallurgical and Materials Transactions*, vol. 27A, pp. 441- 450 (1996).
- Johnson, J.L. and German, R.M., Solid-state sintering in the presence of a liquid phase. *Sintering Technology*, R.M. German, G.L. Messing and R.G. Cornwall (eds), Marcel Dekker, New York, NY, pp. 237-244 (1996).
- Johnson, J.L. and German, R.M., Solid state contributions to densification during liquid phase sintering. *Metallurgical and Materials Transactions*, (1996).
- Liu, Y. and German, R.M., Contact angle and solid-liquid-vapor equilibrium. *Acta Materialia*, vol. 44, pp. 1657-1663 (1996).
- Liu, Y. and German, R.M., Contact angle and solid-liquid-vapor equilibrium. *Acta Materialia*, vol. 44, pp. 1657-1663 (1996).
- Liu, Y., and German, R.M., Relationship between contact angle and surface tensions. *Sintering Technology*, R.M. German, G.L. Messing and R.G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 229-2236 (1996).
- Liu, Y., Iacocca, R., Johnson, J.L., German, R.M., and Kohara, S., Microstructural anomalies in a W-Ni alloy liquid phase sintered under microgravity conditions. *Metallurgical and Materials Transactions*, vol. 26A, pp. 2485-2486 (October 1995).
- Liu, Y., Iacocca, R., Johnson, J.L., German, R.M. and Kohara, S., Microstructural anomalies in a W-Ni alloy liquid phase sintered under microgravity conditions. *Metallurgical and Materials Transactions*, vol. 26A, pp. 2485-2486 (October 1995).

Proceedings

Bose, A., and German, R.M., "Developments in the sintering of Tungsten heavy alloys." Proceedings of the Sintering Technology, R. M. German, G. L. Messing and R. G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 269-276, 1996.

German, R.M., "The microstructures of liquid phase sintered materials." Proceedings of the Sintering Technology, R.M. German, G.L. Messing and R.G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 213-220, 1996.

Iacocca, R.G., Liu, Y., and German, R.M., "Microstructural examination of Tungsten heavy alloys sintered in a microgravity environment." Proceedings of the Advances in Powder Metallurgy and Particulate Materials, vol. 1, Metal Powder Industries Federation, Princeton, NJ, pp. 4.239-4.249, October 1995.

Johnson, J.L., and German, R.M., "Solid-state sintering in the presence of a liquid phase." Proceedings of the Sintering Technology, R.M. German, G.L. Messing and R.G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 237-244, 1996.

Johnson, J.L., Upadhyaya, A., and German, R.M., "Effect of solubility on shape retention during liquid phase sintering." Proceedings of the Advances in Powder Metallurgy and Particulate Materials, vol. 1, Metal Powder Industries Federation, Princeton, NJ, pp. 4.219-4.228, October 1995.

Liu, Y. and German, R.M., "Relationship between contact angle and surface tensions." Proceedings of the Sintering Technology, R.M. German, G.L. Messing and R.G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 229-2236, 1996.

Liu, Y., Iacocca, R.G. and German, R.M., "A challenge to liquid phase sintering concepts." Proceedings of the Advances in Powder Metallurgy and Particulate Materials, vol. 1, Metal Powder Industries Federation, Princeton, NJ, pp. 4.199-4.208, October 1995.

Presentations

German, R.M., "The microstructures of liquid phase sintered materials." presented at Sintering 1995, Penn State University, University Park, PA, September 25, 1995.

German, R.M., "Gravitational effects in liquid phase sintering." submitted presentation, 1996 TMS Annual Meeting, Anaheim, CA, February 6, 1996.

German, R.M., "Recent advances in liquid phase sintering." invited colloquium, Department of Materials Science and Engineering, Case Western Reserve University, Cleveland, OH, April 1, 1996.

German, R.M., "Sintering processes in novel manufacturing systems." invited presentation, Institute of Mechanics and Materials, University of California, San Diego, CA, May 14, 1996.

German, R.M., "The gravitational role in liquid phase sintering." presented at the Microgravity Materials Science Conference, Huntsville, AL, June 11, 1996.

Isothermal Dendritic Growth Experiment**PRINCIPAL INVESTIGATOR:** Prof. Martin E. Glicksman**Rensselaer Polytechnic Institute****CO-INVESTIGATORS:**

No Co-I's Assigned to this Task

Task Objective:

Continue analysis of the resulting space flight and terrestrial data from the Isothermal Dendritic Growth Experiment (IDGE) on its first Space Shuttle mission (STS-62), as apart of the Second United States Microgravity Payload (USMP-2). Determine dendritic tip velocity and tip radius as functions of supercooling. Use velocity and radius data to evaluate the validity of theoretical models that purport to predict velocity and radius. These models are used to improve industrial metal production on Earth. We will publish reports and present papers to inform the scientific community of our findings.

Operate the IDGE space experiment during the second flight of IDGE aboard USMP-3 on STS-75 in February 1996. Acquire and analyze both terrestrial and space data gathered at three different supercoolings in order to characterize the three-dimensional shape of dendritic tips.

Acquire and analyze space data gathered at elevated microgravity levels to determine the effect of residual microgravity on the size, shape, speed, and orientation of dendritic growth.

Develop the first microgravity experiment operations center at a United States university. Demonstrate the ability to command and control a microgravity space experiment from a Principal Investigator's home site.

Work on upgrades which are required for the third flight of IDGE aboard USMP-4, currently scheduled for late 1997. The scientific objectives of the third flight are similar to the first and second flights, but utilize a different sample material. We will modify the IDGE apparatus to accommodate the use of Pivalic Acid as the new sample material.

Task Description:

The Isothermal Dendritic Growth Experiment is a fundamental Materials Science Experiment performed on the Space Shuttle. The specific topic is dendritic solidification which is relevant to virtually all industrial manufacturing of metals and alloys on Earth.

The second flight of IDGE was performed in the cargo bay of the Space Shuttle using an apparatus designed, built, and tested at the NASA Lewis Research Center in Cleveland, Ohio, USA. Over 400 photographs of dendrites that solidified in space along with over 800 photographs of dendrites solidified on Earth were produced on the second flight (STS-75). Each photograph was accompanied by 8 or more scientifically important measurements of time, temperature, and local acceleration. While in space, the apparatus was operated by IDGE personnel located in the Payload Operations Control Center (POCC) at the George C. Marshall Space Flight Center (MSFC) in Huntsville, Alabama, the Teleoperations Support Center at the Lewis Research Center, and at Rensselaer Polytechnic Institute (RPI).

During the STS-75 mission, LeRC and RPI personnel worked together to analyze the IDGE CCD camera dendrite images which are transmitted down to earth in near real time, in order to replan the remaining portion of the mission.

After the flight, RPI personnel will analyze the resulting 35 mm photographs and other data to determine the dendrite tip velocity, as well as characterize the three-dimensional size and shape of the dendrite tip. This data will be used to assess the validity of various solidification theories which are currently being used to try to improve industrial metal production on Earth.

RPI personnel will publish reports and give papers at relevant conferences to disseminate the information to the scientific and industrial community.

Task Significance:

IDGE will study dendrites. Dendrites are tiny crystalline structures that form inside molten metals and metal alloys when they solidify. Nearly all industrially important metals solidify dendritically from the molten state. The dendrites formed inside metals during manufacturing result in microscopic zones of strength, weakness, ductility, and brittleness. Consequently, understanding precisely how dendrites form can lead to improvement of alloy strength and ductility by eliminating weak and brittle areas in the metal. Metal products can be improved, while lowering production costs.

During the past 50 years, numerous scientists have attempted to develop practical theoretical models to predict important dendritic growth parameters. However, years of experimentation on Earth has not produced a data set capable of testing the models to find out which one, if any, is correct. This is due to the influence of gravity.

On Earth, dendritic solidification can be strongly affected by gravitationally driven convective currents in the molten metal. These currents exist during virtually all metal solidification processes. However, their effect on dendritic solidification cannot be accurately be modeled without knowledge of dendritic solidification in the absence of such currents.

The microgravity environment of space effectively eliminates convection in the IDGE experiment. Extensive non-advocate peer review indicated that a comparison between space experiment data and Earth experiment data is the only practical way to separate the effects of convection from the underlying mechanism of dendritic solidification.

Ultimately, IDGE may result in the improved industrial manufacturing of steel, aluminum, super alloys, and other metals that are used on Earth every day. Moreover, the data returned from space will remain relevant indefinitely. IDGE data can be used to test current theories, as well as theories that will be developed perhaps far into the future. In fact, the Schriber Committee report (1987) declared that the IDGE was one of NASA's four "world-class" microgravity science experiments due to the quality, scope, and long term relevance of its science.

Progress During FY 1996:**First Flight of IDGE**

The Isothermal Dendritic Growth Experiment (IDGE) is a tele-operated microgravity science experiment payload that flew on the space shuttle Columbia in March of 1994. The first mission was an unqualified success. Analysis of the flight data revealed that current solidification theories need significant modification. Personnel at RPI have concluded all the analysis of the data from the first mission.

Second Flight of IDGE

The IDGE apparatus was operated successfully for 15 days aboard STS-75 during February/March 1996. The IDGE apparatus had been significantly modified in order to achieve and even surpass the science requirements for the second flight. The most important modification was the installation of an autofocus system for the 35 mm cameras. In addition, the Slow Scan Television cameras were replaced with higher resolution CCD cameras, which transmitted images down to Earth in near real time. These images were analyzed immediately, and the information gathered was used to alter the experiment protocol for the remaining portion of the mission.

Initial analysis of the downlinked data indicates that the residual microgravity environment of space does not affect the size, shape, speed, or orientation of dendritic growth, as was previously theorized.

Analysis of the 35 mm photographs has just begun.

A fully functional remote operations center was set up at Rensselaer Polytechnic Institute for the STS-75 mission. The IDGE was the first microgravity space experiment commanded and controlled from a United States university. The Rensselaer Operations and Control Center became the primary site of operations for the last 5 days of the mission. This yielded invaluable insight into the world of remote telescience, whereby principal investigators are able to stay at the university and operate their experiment, thus eliminating the need to travel to a NASA center to accomplish the scientific objectives of their research. This proof of concept demonstration was an unqualified success. This demonstration was vitally important as this is the prevailing operations concept currently being developed for the upcoming International Space Station era.

Third Flight of IDGE

In order to achieve the science objectives for the third flight of IDGE aboard USMP-4 on STS-87, currently scheduled for October 1997, significant modifications must be made to the apparatus. A different sample material will be used to grow dendrites. The current growth chamber design may be inadequate to accomplish this objective. Therefore, in addition to producing several growth chambers of the current design, a new all glass growth chamber has been designed and fabricated, filled and tested. All glass flight models are being fabricated.

Recent developments in the field have indicated that there may be dynamic oscillations of the edge of dendrites as they grow. A video cassette recorder is being installed into the IDGE flight unit in order to video tape the dendritic growths. The video will also be downlinked to the ground during the mission.

RPI personnel have improved their techniques required to purify pivalic acid (PVA), the sample material to be used in the third flight. RPI now has now filled several engineering growth chambers.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	13	BS Degrees:	0
MS Students:	6	MS Degrees:	1
PhD Students:	5	PhD Degrees:	0

TASK INITIATION: 12/88 EXPIRATION: 12/98

PROJECT IDENTIFICATION: 963-25-05-01

NASA CONTRACT NO.: NAS3-253

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Bushnell, L.T., Koss, M.B., LaCombe, J.C., and Glicksman, M.E., Use of microgravity to interpret dendritic growth kinetics at small supercoolings. *J. Crystal Growth*, (submitted 1996).

Koss, M.B., Bushnell, L.T., LaCombe, J.C., and Glicksman, M.E., The effect of convection on dendritic growth under microgravity conditions. *Chem. Eng. Comm.*, (in press 1996).

LaCombe, J.C., Oudemool, J.L., Koss, M.B., Bushnell, L.T., Bushnell, and Glicksman, M.E., Measurement of thermal expansion in liquid succinonitrile and pivalic acid. *J. Crystal Growth*, (in press 1996).

Proceedings

Glicksman, M.E., "Convective effects in microgravity on dendritic growth kinetics and morphology." 34th Aerospace Sciences Meeting and Exhibit, Reno, NV, January, 1996.

Glicksman, M.E., Koss, M.B., Bushnell, L.T., LaCombe, J.C., and Winsa, E.A., "Dendritic growth measurements in microgravity." *Lecture Notes in Physics*, vol. 464, Eds. L. Ratke, H. Walter, and B. Feuerbacher, (Springer-Verlag, Berlin, p. 63, 1996).

Glicksman, M.E., Koss, M.B., Bushnell, L.T., LaCombe, J.C., and Winsa, E.A., "Convective effects in microgravity on dendritic growth kinetics and morphologies." Paper # AIAA 96-0251, Aerospace Sciences Meeting and Exhibit, Reno, NV, 1996.

LaCombe, J.C., Koss, M.B., Bushnell, L.T., de Jager, K.D., and Glicksman, M.E., "Dendrite tip shape characteristics." *Mat. Res. Soc. Symp. Proc.* (Materials Research Society, Pittsburgh, PA, in press 1996).

Schiffman, R.A., "Development of a university based remote teleoperations site for the performance of experiments in microgravity." 8th International Symposium on Experimental Methods for Microgravity Materials Science, (The TMS, Warrendale, PA, in press 1996).

Presentations

Glicksman, M.E., "Dendritic growth studies on the space shuttle." Science Update, at the Sixth Eastern Regional Conference on Crystal growth, ACCG/east-95, in Atlantic City, NJ, October, 1995.

Glicksman, M.E., "The experimental measurement of the thermal expansion of liquid succinonitrile." October meeting of the Mohawk chapter of the TMS, October, 1995.

Glicksman, M.E., "Development of a university based local teleoperations site for the performance of experiments in microgravity." 8th International Symposium on Experimental Methods for Microgravity materials Science at the 5th TMS Annual Meeting, Anaheim, CA, February, 1996.

Glicksman, M.E., "Diffusion-limited dendritic growth." Current Status and Recent Microgravity Results, Chemical Engineering Seminar, University of Florida, April, 1996.

Glicksman, M.E., "Experience with a materials microgravity space flight experiment." URI Composite Materials Program, Rensselaer Polytechnic Institute, Troy, NY, April, 1996.

Glicksman, M.E., "Study of dendritic crystal growth in microgravity using teleoperational control." Space Processing of Materials, SPIE's 1996 International Symposium on Optical Science, Engineering, and Instrumentation, Denver, CO, August, 1996.

Glicksman, M.E., "Use of microgravity to interpret dendritic growth kinetics at small supercoolings." Tenth American Conference on Crystal Growth (ACCG-10), Vail, CO, August, 1996.

J.C. LaCombe, J.C., "Dendrite tip shape characteristics." Material Research Society Fall '95 Conference, Symposium C, December, 1995.

Koss, M.B., "The isothermal dendritic growth experiment." Microgravity Materials Science Conference, Huntsville, AL, June, 1996.

M.E. Glicksman, M.E., "The isothermal dendritic growth experiment on the space shuttle Columbia, The Japan Institute of Metals." International Symposium on Advanced Materials & Technology for the 21st Century, Honolulu, Hawaii, December, 1995.

M.E. Glicksman, M.E., "The isothermal dendritic growth experiment: space flight results from USMP-2 (1994), and USMP-3 (1996)." Lecture 2, 1996 Summer School on Pattern Formation, Interfacial Dynamics, and Crystal Growth, Toledo, Spain, May, 1996.

Physical Properties and Processing of Undercooled Metallic Glass Forming Liquids

PRINCIPAL INVESTIGATOR: Dr. William L. Johnson

California Institute of Technology (Caltech)

CO-INVESTIGATORS:

Lee, D.S.

Amorphous Technologies International

Task Objective:

The objective is to study the specific heat, thermal conductivity, density, and viscosity of undercooled glass forming metallic alloy melts. Heat capacity and thermal conductivity measurements are accomplished by the use of the AC Modulation Calorimetry as implemented on the TEMPUS facility in the MSL-1 flight. The data to be obtained are essential for the understanding of the thermodynamic and kinetic aspects of glass formation in alloys as well as the development of advanced processing technology for glass forming metals.

Task Description:

Non-contact ACOM measurements were successfully demonstrated in the TEMPUS facility during the IML-2 shuttle flight in July 1994. Specific heat and thermal conductivity data were obtained for the glass forming alloys $Zr_{76}Ni_{24}$ and $Nb_{40}Ni_{60}$ using the TEMPUS facility. The data have been analyzed to obtain the heat capacity and effective thermal conductivity of these liquids at a sequence of temperatures. These results, in turn, have been used to compute the entropy and free energy functions of the liquid alloys. The IML-2 experiment was plagued by cross-contamination problems between the samples of the six investigators, the ceramic components in the sample holders, etc. Further problems with sample stability hampered the IML-2 experiments. As a result of the contamination problems, limited undercooling of the liquids was achieved. The stability and contamination problems with TEMPUS have been addressed and corrected for the MSL-1 flight.

Samples to be studied in the MSL-1 flight include: Zr-Ni, Zr-Ni-Cu, and Zr-Ti-Ni-Cu alloys. Sample characterization and parameter sets for the ACOM experiments are being developed in collaboration with the MUSC group in Cologne using the "breadboard" TEMPUS model. Ground-based measurements of total hemispherical emissivity of these samples are being carried out at Caltech using an electromagnetic levitator and total radiance bolometer.

Task Significance:

The ACOM method provides accurate specific heat data (2 - 4% accuracy) and thermal conductivity data for high temperature reactive liquid alloys for which ground-based methods requiring a container are inapplicable. In this regard, the ACOM technique is a "benchmark" for heat capacity studies of reactive liquids. Data in both the equilibrium and undercooled liquid states can be obtained. Maximum undercooling is achievable with the use of a containerless measurement. These data are essential for scientific understanding of glass formation and crystal nucleation (in the undercooled state) for these materials. Further, the data provide a basis for modeling the processing of these materials for commercial applications. The alloys under study belong to a sequence of alloys which exhibit progressively enhanced glass forming ability. The more complex quaternary alloys are of commercial interest for casting of three dimensional metallic glass components. The data obtained from the flight experiment will provide a basis for developing commercial processing methods.

Progress During FY 1996:

Samples to be studied on the TEMPUS facility during the MSL-1 mission have been selected. Specimens for parameter evaluation on the TEMPUS "breadboard" model have been delivered to DLR for preliminary parameter determination. D. Lee and S. Glade will spend a week at DLR in October/November to carry out detailed parameter set determination for the Caltech samples. The alloys to be studied were jointly selected by the Fecht/Wunderlich group (Berlin) and the Johnson/Lee group (Caltech) to optimize the potential results of the overall project. These samples include:

- 1) elemental Zr (Hoffmeister sample, to be studied by Johnson/Lee)
- 2) $Zr_{64}Ni_{36}$ (Fecht/Wunderlich)
- 3) $Zr_{60}Ni_{20}Cu_{20}$ (Johnson/Lee)

- 4) $Zr_{10}Ti_{34}Ni_8Cu_{48}$ (Johnson/Lee)
- 5) $Zr_{65}Ni_{10}Cu_{15}Al_{10}$ (Fecht/Wunderlich)
- 6) Zr-Ti-Ni-Cu-Al (Johnson/Lee)
- 7) Zr-Co-Ni-Cu-Al (Fecht/Wunderlich)

These alloys represent a series of alloys with progressively enhanced glass forming ability and potential for undercooling. Ground-based experiments have been carried out on the Caltech samples. These include differential scanning calorimetry measurements of the specific heat of the solid glassy samples at temperatures below T_g as well as DSC measurements in the undercooled liquid region immediately above T_g (temperatures up to 100 K above T_g). To determine the processability of the undercooled liquid at higher temperatures (below, near, and above the equilibrium liquidus temperature of the alloys), we have carried out ground-based undercooling studies using the High Temperature High Vacuum Electrostatic Levitation (HTHVESL) facilities at JPL (in collaboration with Dr. W.Q. Rhim) and at Loral Space Systems (Palo Alto, California, in collaboration with Drs. John Watkins and A. Rulison). These studies have allowed us to develop time-temperature-transformation diagrams describing the onset of crystallization for the undercooled liquid alloys. These data are then used to develop appropriate time-temperature profiles for the MSL-1 AC Modulation Calorimetry experiments. Ground-based determination of the optical constants for the samples including spectral emissivity and total hemispherical emissivity are also being carried out using the HTHVESL ground-based facilities. These data will be required for analysis of MSL-1 results.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/95 EXPIRATION: 7/99

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NAG9-119

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Kim, Y.J., Busch, R., Johnson, W.L., Rulison, A.H., and Rhim, W.Q. Experimental Determination of a Time-Temperature-Transformation Diagram of the Undercooled $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ Alloy Using Containerless Electrostatic Levitation Processing. *Appl. Phys. Lett.*, vol. 68, 1057-1059 (1996).

Wunderlich, R.K., Lee, D.S., Johnson, W.L., and Fecht, H.J. Non Contact Modulation Calorimetry of Metallic Liquids in Low Earth Orbit. *Phys. Rev. B, Rapid Commun.* (1996).

Proceedings

Busch, R., Kim, Y.J., Schneider, S., and Johnson, W.L. "Atom Probe Field Ion Microscope and Levitation Studies of the Decomposition and Crystallization of Undercooled Zr-Ti-Cu-Ni-Be Melts." *ISMANAM-95 Conference Proceedings*, Materials Forum, 77-82 (1996).

Johnson, W.L. "Fundamental Aspects of Bulk Metallic Glass Formation in Multicomponent Alloys." *Proceedings of ISMANAM-95*, R.S. Schulz, ed., Materials Forum, 35-49 (1996).

Kim, Y.J., Busch, R., and Johnson, W.L. "Crystallization Kinetics of the Undercooled Liquid $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ Alloy During Containerless Electrostatic Levitation Processing." *8th Int. Symp. of Experimental Methods for Microgravity Materials Science*, TMS, R.A. Schiffman, ed., in press (1996).

Lee, D.S., Hoffmeister, W., Bayuzick, R., and Johnson, W.L. "Noncontact AC Calorimetry: Specific Heat of Liquid $Nb_{40}Ni_{60}$ and $Ni_{74}Zr_{26}$ as Measured on IML-2." *Thermophysical Journal, Proc. of the 4th Asian Thermophysical Properties Conference*, 884-888 (1995).

Thermophysical Properties of Metallic Glasses and Undercooled Alloys

PRINCIPAL INVESTIGATOR: Dr. William L. Johnson

California Institute of Technology (Caltech)

CO-INVESTIGATORS:

Lee, D.S.

Amorphous Technologies International

Task Objective:

The objective is to study thermophysical properties of undercooled alloy melts and how they relate to glass formation. Toward this end, we have developed non-contact calorimetric methods to investigate the specific heat and thermal conductivity of these melts, both in the liquid and undercooled region. These quantities are essential for the development of newer, more advanced processing technologies for both existing and future materials.

Task Description:

Non-contact AC calorimetry was successfully demonstrated on the IML-2 flight in July, 1994. We obtained information on the specific heat and thermal conductivity of liquid and undercooled $Zr_{76}Ni_{24}$ and $Ni_{60}Nb_{40}$ melts using TEMPUS. This data is currently being analyzed to calculate entropy and free energy functions for these melts. We will compare these quantities to their values for the corresponding equilibrium and metastable crystals to compare the relative stability of the phases. Also, we will determine the Kauzman isentropic temperature of the alloys and compare it to the observed glass transition temperature.

In addition, the ground-based total radiance bolometer is currently being integrated onto a UHV levitation chamber for total hemispherical emissivity measurements. Measurement of temperature-dependent total hemispherical emissivity functions will allow us to unwind specific heat from undercooling data in an unambiguous manner.

Task Significance:

The non-contact AC calorimetry experiment is significant for many reasons. First, the thermodynamic properties of these advanced materials are a prerequisite to the development of processing technologies for them. Without knowledge of heat capacities and thermal conductivities, it is not possible to define, for example, how much power is needed to melt and cast the materials. In addition, the specific materials chosen for our experiment are the parent compounds for a new class of bulk metallic glasses that have recently been discovered by our group here at Caltech. By studying the properties of these parent compounds, we hope to better understand the bulk metallic glasses and how they form. These materials will revolutionize metallic processing technologies with their novel, superior properties. These materials can be engineered to be more ductile, slipperier, harder, lighter and more corrosion resistant than the typical materials used today. It is essential that the processing technologies for these materials be developed as quickly as possible and that, therefore, the thermophysical properties be measured.

Progress During FY 1996:

The final report for this project was submitted in September 1996. The flight data obtained on TEMPUS during the IML-2 mission have been analyzed and the results of ACMC measurements carried out during IML-2 have been reported in a number of meetings and submitted for publication in journals as reported in the bibliography section. In addition to the IML-2 results, we have carried out ground-based studies of the glass forming liquid alloys using the High Vacuum Electrostatic Levitation method in collaboration with Dr. W.Q. Rhim's group at JPL. This work was carried out by Dr. Y.J. Kim and was used to provide ground-based support for the flight experiments. In particular, undercooling studies, and crystal nucleation kinetics vs. undercooling have been measured for the glass forming alloy samples of this study using the ground-based Electrostatic Levitation facility at JPL, while ground-based heat capacity measurements (using DSC at Caltech) were carried out to provide a data base for comparison with results of the flight experiments.

The ACMC method is constantly being refined. Better filtering and analysis routines have been developed and used to analysis data from IML-2. A ground-based electromagnetic levitation facility for use in measuring total hemispherical emissivity was built under support of this grant and is operational. It is being used to characterized the flight samples for both the IML-2 and upcoming MSL-1 missions.

We summarize the heat capacity data obtained from the IML-2 flight experiment on one of the best analyzed IML-2 binary alloy samples, $Zr_{64}Ni_{36}$, in the table below. The data were analyzed using the method of sample impedance change during melting as described by Wunderlich *et. al.* (Phys. Rev. B, Rapid Comm., in press, 1996) to determine the power coupling constant to the sample.

Table. Specific heat data for liquid $Zr_{64}Ni_{36}$ obtained from IML-2 mission.

Temperature (C)	Mod. Freq. (Hz)	Total Hemispherical Emissivity	Heat Capacity (J/mole-K)
1215	0.05	0.37	43.7 +/- 0.8
1160	0.08	0.35	44.5 +/- 1.2
	0.10	0.35	43.2 +/- 1.0
1038	0.05	0.33	43.9 +/- 1.0
	0.08	0.33	44.2 +/- 1.0
1008	0.05	0.32	44.0 +/- 1.0
	0.10	0.32	44.6 +/- 1.0
980	0.05	0.32	45.5 +/- 1.2

The development of the ACMC method is being continued and refined as part of another round of experiments to be carried out on the TEMPUS facility during the upcoming MSL-1 shuttle flight. The continuing work is supported under NASA Grant. No. NAG9-1192.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0 BS Degrees: 0
MS Students: 2 MS Degrees: 0
PhD Students: 2 PhD Degrees: 1

TASK INITIATION: 2/92 EXPIRATION: 4/98

PROJECT IDENTIFICATION: 963-35-10

NASA CONTRACT NO.: NAG8-954

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Busch, R., Kim, Y.J., Johnson, W.L., Rulison, A.J., and Rhim, W.Q. Total hemispherical emissivity and specific heat capacity of deeply undercooled $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ melts. Appl. Phys. Lett., vol. 66, 3111-3113 (1995).

Lee, D.S., Uffelman, D., and Johnson, W.L. Noncontact AC calorimetry on undercooled alloys: Science and technology of rapid solidification and processing. NATO ASI Series E - Applied Sciences (M. Otonari, ed.), vol. 278, 327-337 (1995).

Proceedings

Busch, R., Kim, Y.J., Johnson, W.L., Rulison, A.J., and Rhim, W.K. "Determination of the specific heat capacity and the total hemispherical emissivity of the deeply undercooled $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ alloy." Proc. of the 7th Int'l. TMS Symposium on Experimental Methods for Microgravity Materials Science, TMS, 15-21 (1995).

Orbital Processing of High Quality Cadmium Telluride

PRINCIPAL INVESTIGATOR: Prof. David J. Larson, Jr.

State University of New York, Stony Brook

CO-INVESTIGATORS:

Dudley, M.
Gillies, D.
Alexander, J.I.D.
Carlson, F.M.
Moosbrugger, J.
DiMarzio, D.

SUNY at Stony Brook
NASA Marshall Space Flight Center (MSFC)
University of Alabama, Huntsville (UAH)
Clarkson University
Clarkson University
Northrop Grumman ATDC

Task Objective:

The objective of this research is to investigate the influences of gravitationally-dependent phenomena (hydrostatic and buoyant) on the growth and quality of doped and alloyed Cadmium-Zinc-Telluride (CdZnTe) crystals grown by the modified seeded Bridgman-Stockbarger technique. It is hypothesized that the damping of the gravitationally-dependent buoyancy convection will substantially enhance chemical homogeneity and the near-elimination of hydrostatic pressure will enable significant reduction in defect (dislocations and twins) density.

Task Description:

The primary objective of this program is to grow CdZnTe crystals in orbit (μ -g) for comparison with the best crystals grown terrestrially (1-g). Our comparative baseline includes crystals grown within the program and at the best commercial facilities. Our hypothesis suggested that crystals grown in μ -g could be grown under diffusion controlled growth conditions, due to the damping of gravitationally-dependent convective (buoyant) flows. Further, in the near-absence of hydrostatic pressure in μ -g, crystals could be grown virtually without melt/crystal/ampoule wall contact. It was hypothesized that this would significantly reduce the thermo-mechanical stresses experienced by the growing and cooling crystal and improve the defect density (twins and dislocations) of the resulting CdZnTe crystals.

As a critical part of this task, two crystals were grown in μ -g using the seeded Bridgman-Stockbarger growth technique on USML-1 (STS-50) in 1992, and two additional crystals were processed on USML-2 (STS-73) in 1995. The seeded Bridgman-Stockbarger crystal growth technique, is accomplished by establishing isothermal hot zone and cold zone temperatures that bracket the solidification temperature (1095 °C) with a uniform thermal gradient in between. After sample insertion into the Crystal Growth Furnace (CGF) the furnace's hot and cold zones are ramped to temperature, establishing a thermal gradient of 35 °C/cm and melting the bulk of the sample. The furnace is equilibrated and then moved back towards the seed crystal, causing the bulk melt to come in contact with the seed crystal, seeding the melt. The seed crystal prescribes the growth orientation of the crystal grown. Having seeded the melt, the furnace is re-equilibrated, furnace translation is reversed, and the sample is solidified directionally by passing the thermal gradient down the length of the sample at a uniform velocity (1.6 cm/h).

Task Significance:

The family of II-VI compound semiconductors, of which CdZnTe is a commercially significant member, is used in the fabrication of medium and long wavelength IR sensors and beta and gamma ray nuclear detectors. Orbital processing offers a unique opportunity to advance toward the goal of greatly increased structural perfection within bulk crystals of increased chemical homogeneity, by growing, characterizing, and testing paradigm material. Further, seeding technologies are being developed which will be useful to industry, and insight will be generated with respect to the generation of twins, which are pervasive terrestrially and greatly reduce the yield of II-VI bulk crystal growth efforts.

Progress During FY 1996:

Three (3) of the above crystals, two (2) on USML-1 (FY92) and one (1) on USML-2 (FY96), were grown using a standard Bridgman-Stockbarger seeded growth configuration with a 6 mm diameter seed crystal, and a 15 mm diameter bulk crystal with a shoulder between. The sample on USML-2 had an internal spring which constrained

the liquid during growth, enforcing wall contact. The fourth sample was processed on USML-2 in an identical manner thermally, and with the same seed geometry. The ampoule, however, was designed with a continuous taper instead of a shoulder, to minimize wall contact between the growing and solidifying crystal and the ampoule. This was intended to maximize the volume of material which solidified without wall contact. The absence of wall contact was of particular interest since it had been shown to minimize thermo-mechanical stresses experienced by the crystal during growth and post-solidification cooling, with concomitant defect reduction. This experiment could only be attempted in μ -g where there is a near-absence of hydrostatic pressure on the bulk liquid.

It was found that the chemical homogeneity of the crystals grown in μ -g was outstanding longitudinally and radially. This suggested that gravitationally-dependent thermosolutal convection had been damped and diffusion-controlled growth had been achieved, as anticipated by our high fidelity process model. This result also suggests that in this alloy system surface driven convection is not a significant detriment to the attainment of diffusion-controlled growth conditions in microgravity. Chemical mapping of these samples will continue into FY97.

The experiments on USML-1 demonstrated that in the near-absence of hydrostatic pressure the non-wetting liquid separated from the ampoule walls, as proposed, depending on influences including: volumetric fill-factor, residual g-vector, ampoule geometry and growth conditions. The standard USML-2 sample demonstrated an effective liquid constraint technique, generating a sample solidified with full wall contact. The latter sample demonstrates surface strains and twin densities that are typical of ground samples. Regions solidified without wall contact were found to virtually eliminate twinning, suggesting that these pervasive defects terrestrially are largely surface nucleated. Further, regions without wall contact showed dramatic reductions in (111)[110] dislocation density, from 800,000 (1-g) to 800 (μ -g) epd. This should also be compared to typical best commercial products averaging 30,000 epd. Improvement resulted from reduced thermo-mechanical stress within the flight samples during growth and post-solidification cooling. Regions of partial wall contact showed defect gradients, with high densities on the wall side and low densities on the free surface side. These results are consistent with output from the high-fidelity thermal and thermo-mechanical stress model. Quantitative analysis of these samples will continue into FY97.

Lastly, the tapered ampoule successfully extended the region of regrowth without wall contact to 22 mm, followed by partial wall contact for an additional 28 mm. Surface analysis using optical microscopy and x-ray synchrotron topography confirmed the absence of twinning in the freely grown region and the reappearance of twinning with wall contact. Further, the topographs suggest a very low strain content, suggesting that this will prove to be very low in [110](111) dislocation density. Analysis of these samples will continue into FY97.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	4
PhD Students:	2	PhD Degrees:	3

TASK INITIATION: 8/90 **EXPIRATION:** 12/96**PROJECT IDENTIFICATION:** 963-21-08-02**NASA CONTRACT NO.:** NAS8-397**RESPONSIBLE CENTER:** MSFC

Orbital Processing of Eutectic Rod-like Arrays (OPERA)

PRINCIPAL INVESTIGATOR: Prof. David J. Larson, Jr.

State University of New York, Stony Brook

CO-INVESTIGATORS:

Dudley, M.

Favier, J.J.

Alexander, J.I.D.

State University of New York at Stony Brook
C.E.N.G. (France)

University of Alabama at Huntsville (UAH)

Task Objective:

The objective of this program is to utilize the orbital microgravity environment to conduct unique experiments to evaluate process models that describe convective influences on solidification of regular, low volume fraction, eutectic alloys.

Task Description:

The primary objective of this program is to directionally solidify regular eutectic structures in orbit (μ -g), while applying complementary in-situ diagnostics to monitor and perturb the solidification interface velocity and to precisely monitor the temperature at the solidification interface (undercooling). Post-flight analyses will determine, quantitatively, the relations between the velocity, interface temperature (undercooling), and structural parameters. Identical experiments will be conducted terrestrially, under damped (thermal stabilization and applied magnetic fields) and undamped conditions.

As a critical part of this task, a directional solidification model will be developed and validated experimentally with concomitant thermoelectric interface demarcation. This model will include all of the thermoelectric contributions; Peltier, Thomson, Joule, and Seebeck and will predict the eutectic rod-like structure within the pulsed region and within the post-pulse transient. This model will also incorporate Soret diffusion, and convective contributions. A separate effort will be made to modify the Jackson-Hunt theory to include kinetic undercooling and the possibility that the interfacial composition is not the same as the bulk liquid composition.

Task Significance:

Eutectic alloys dominate the brazing and soldering industries. Further, the faceted/non-faceted structures under investigation are descriptive of the microstructures in graphitic steels and cast irons. Obviously, it is important to understand the solidification of these materials since they are of great significance commercially. The dominant theory that describes eutectic solidification, that of Jackson and Hunt, was derived for diffusion-controlled growth, which is atypical terrestrially since gravitationally-driven convection is pervasive. Prior analytical convective sensitivity tests of this theory predicted convective insensitivity. Directional solidification experiments under damped (microgravity or magnetic field) conditions have demonstrated a significant sensitivity, challenging this fundamental theory. This program addresses this conflict experimentally and analytically.

Progress During FY 1996:

An advanced in-house numerical program, MASTRAPP, has been modified to include a complete description of the thermoelectric effects (Peltier, Thomson, Joule and Seebeck) which contribute to the thermal perturbations that result in interface demarcation. This program uses a non-orthogonal curvilinear coordinate system and a multi-zone adaptive grid generation scheme and dynamically simulates Bridgman-Stockbarger Crystal Growth with concomitant Interface Demarcation. The program will be further expanded to include compositional redistribution, including Soret and electrotransport contributions, as well as convection.

The code is operational and has been applied to the case of pure Bismuth, which is the dominant species in the Bi-MnBi eutectic system under evaluation. Interface shapes and locations, as well as the velocity and acceleration environments that the growing crystal experiences during the transients associated with current pulsing have been modeled. Qualitatively, the transient velocities and sequences predicted have been validated from a prior data archive, and a specific matrix of experiments is being conducted to validate the code experimentally.

Two small NASA furnaces have been transferred to the SUNY-SB solidification laboratory from the University of Alabama in Birmingham. These furnaces have been installed and thermal and velocity calibrations have been initiated. New programmable electronics have been acquired to control the interface demarcation experiments and a computer system has been acquired to apply Lab View to overall experiment control and data acquisition and display.

Ampoules and thermal loads, with and without interface demarcation leads, have been designed and ampoules are in fabrication. High purity materials have been ordered and alloy fabrication will be initiated in November. Prior stock will be utilized until new materials are available.

Discussions have been initiated with CENG, France to determine whether the French flight furnace MEPHISTO is an appropriate experimental vehicle for this experiment. Two meetings have been held to date. Preliminary evaluation suggests that MEPHISTO is capable of hosting this experiment, but the question of its availability is still open. Experiments that would introduce Seebeck eutectic measurements to this program have been thoroughly discussed and experiments are planned to be conducted in 1997 in both the CENG MEPHISTO prototype furnace and at the University of Florida. Further, experiments with applied magnetic field damping have been planned for summer 1997 at the Space Sciences Laboratory at the Marshall Space Flight Center. These opportunities will substantially expand the one-g data base that will be developed at SUNY-SB.

It is anticipated that interface demarcation observation will be conducted using optical microscopy, with and without differential etching. X-ray Synchrotron Topography has been successfully applied by our topography group to reveal Peltier melt-back, and change-of-rate interfaces. X-ray techniques will be investigated as a means of revealing interface demarcation within eutectic systems in the coming year.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/96 EXPIRATION: 11/99

PROJECT IDENTIFICATION:

NASA CONTRACT No.: NCC8-100

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Fedoseyev, A., and Alexander, J.I.D. An Inverse Finite Element Method for Pure and Binary Solidification Problems. J. Computational Physics, (1996, accepted).

Moosbrugger, J.C. Continuum Slip Viscoplasticity with the Haasen Constitutive Model: Application to CdTe Single Crystal Inelasticity. International Journal of Plasticity, vol. 11, 799 - 826 (1995).

Presentations

Larson, Jr., D.J. "Orbital Processing of High-Quality Zn-Alloyed CdTe Compound Semiconductors." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Crystal Growth of II-VI Semiconducting Alloys by Directional Solidification

PRINCIPAL INVESTIGATOR: Dr. Sandor L. Lehoczky

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Szofran, F.

NASA Marshall Space Flight Center (MSFC)

Su, C.-H.

NASA Marshall Space Flight Center (MSFC)

Scripa, R.

University of Alabama, Birmingham (UAB)

Sha, Y.

Universities Space Research Association (USRA)

Task Objective:

The objective of this research is to investigate the effects of reduced gravity on the crystal growth of mercury zinc telluride (HgZnTe) and mercury zinc selenide (HgZnSe) alloys with respect to their compositional, metallurgical, and optical properties.

Task Description:

The investigation includes both Bridgman-Stockbarger and solvent growth methods, as well as growth in a magnetic field. The alloys are prepared by reacting pure, elemental constituents in evacuated, sealed, fused-silica ampoules. The crystals are grown in a multizone furnace. The hot zone is heated above the liquidus temperature of the given alloy and the cold zone is maintained at lower temperatures to provide temperature gradient sufficient to prevent constitutional supercooling. Crystal growth is accomplished by slowly moving the ampoule from the hot zone to the cold zone of the furnace. The flight portion of the investigation is being performed by using the Crystal Growth Furnace (CGF). Preparation of the samples is being done in the Space Sciences Laboratory of Marshall Space Flight Center. Characterization and analysis of the samples after processing is being done primarily in the same laboratory with substantial microstructural analysis being done at the University of Alabama at Birmingham. Device fabrication and characterization will be done primarily at the Rockwell International Science Center.

Task Significance:

The anticipated results of this study will have both scientific and technological significance. The advancement in science will result from the increased understanding of the role of gravity on the fluid dynamic and compositional redistribution phenomena during the crystal growth of solid-solution semiconducting alloys having large separation between the liquidus and solidus of the constitutional phase diagrams, and from the more accurate values of material properties that can be measured using the high-quality, bulk crystals grown in space. Any advance in quality of these electronic materials has a great technological impact because of the application to infrared detectors for NASA and DOD requirements.

Progress During FY 1996:

Continued the seeded growth of $\text{Hg}_{0.88}\text{Zn}_{0.12}\text{Te}$ and $\text{Hg}_{0.84}\text{Zn}_{0.16}\text{Te}$ crystals by back-melting a series of precast segments and by directional solidification. The predetermined composition profile of these segments simulated the distribution of a "diffusion boundary" layer in the melt ahead of the solid-melt interface during the directional solidification experiments. Composition analysis on the grown crystals confirm that steady-state growths were achieved from the beginning of the growth process. A series of $\text{Hg}_{0.84}\text{Zn}_{0.16}\text{Te}$ crystals were grown vertically by directional solidification in a 5 Tesla axial magnetic field. The ingots were partially grown and quenched to preserve the growth interface shapes. The effects of magnetic damping on the buoyancy-driven convective flows in the melt were investigated by examining the quenched-in interface shapes and by measuring the composition variations along the axial and radial directions of the grown ingots and comparing them with those of ingots grown without a field.

Completed the measurements of the HgTe-ZnTe pseudobinary phase diagram, and melt density and thermal diffusivity as functions of temperature for several alloy compositions. The thermodynamic properties of the melts, such as enthalpy of mixing and specific heat, were calculated for temperatures between the liquidus and 150 °C above the liquidus by assuming an associated solution model for the liquid phase. An oscillating-cup viscometer was used to measure the viscosity for $\text{Hg}_{0.84}\text{Zn}_{0.16}\text{Te}$ melts between 770 and 850 °C. A slow relaxation phenomena

was observed, possibly indicating the presence of subcritical clusters or heterofluctuations near the liquidus temperature.

The intrinsic carrier concentrations, Fermi energies, and the electron effective masses were calculated for $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ with $0 < x \leq 0.4$ and $50\text{K} \leq T \leq 400\text{K}$. The calculations were based on the Kane $k \cdot p$ model and no approximation is made for the energy band structure beyond those inherent in the Kane model. The values obtained were found to be significantly different from previously published results.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	2
MS Students:	1	MS Degrees:	1
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 12/92 EXPIRATION: 9/98

PROJECT IDENTIFICATION: 963-35-05

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Mazuruk, K., Sha, Y.-G., Su, C.-H., and Lehoczky, S.L. Viscosity of $\text{Hg}_{0.84}\text{Zn}_{0.16}\text{Te}$ Pseudobinary Melt. *J. Appl. Physics*, vol. 79(12), 9080-9083 (1996).

Sha, Y.-G., Su, C.-H., Alexander, H.A., Lehoczky, S.L., and Wang, J.-C. Seeded Growth of HgTe-ZnTe by Directional Solidification Using an Initial Composition Profile Simulating a "Diffusion-Boundary" Layer. *J. Crys. Growth* (in press, 1996).

Sha, Y.-G., Su, C.-H., and Lehoczky, S.L. Growth of HgTe-ZnTe by Directional Solidification in a Magnetic Field. *J. Crys. Growth* (in press, 1996).

Sha, Y.-G., Su, C.-H., and Lehoczky, S.L. Intrinsic Carrier Concentrations and Electron Effective Masses in $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$. *J. Appl. Physics* (in press, 1996).

Sha, Y.-G., Su, C.-H., Mazuruk, K., and Lehoczky, S.L. Thermal Diffusivity and Conductivity of HgTe-ZnTe Solids and Melts. *J. Appl. Physics*, vol. 80(2), 752-755 (1996).

Sha, Y.-G., Su, C.-H., Mazuruk, K., and Lehoczky, S.L. Phase Diagram, Density, Heat Capacity and Enthalpy of Mixing Pseudobinary $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ Melts. *J. Appl. Physics*, vol. 80(1), 137-142 (1996).

Proceedings

Lehoczky, S.L., Szofran, F.R., Su, C.-H., Scripa, R.N., and Sha, Y.-G. "Crystal Growth of Selected II-VI Semiconducting Alloys by Directional Solidification." Proceedings of the 1996 Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996 (in press).

Sha, Y.-G., Su, C.-H., Lehoczky, S.L., and Szofran, F.R. "Ground-Based growth of HgTe-ZnTe in a Magnetic Field." Proceedings of the 34th Aerospace Sciences Meeting and Exhibit, Reno, Nevada, January 15-18, 1996 (paper AIAA 96-0256).

Su, C.-H., Gillies, D.C., Szofran, F.R., Watring, D.A., and Lehoczky, S.L. "The Influence of Reduced Gravity on the Crystal Growth of Electronic Materials ("Cooperation in the 21st Century: Advances in Astronautical Sciences")." Proceedings of the 6th International Space Conference of Pacific Basin Societies (6th ISCOPS), P.M. Bainum, G.L. May, Y. Ohkami, K. Uesugi, Q. Faren, and L. Furong, eds., vol. 1, pp 351-363. Marina Del Rey, California, December 6-8, 1995.

Presentations

Sha, Y.-G., Su, C.-H., and Lehoczky, S.L. "Seeded Growth of HgTe-ZnTe by Directional Solidification using Initial Composition Profile Simulating a "Diffusion-Boundary" Layer." The 10th American Conference on Crystal Growth, Vail, Colorado, August 4-9, 1996.

Growth of Solid Solution Single Crystals

PRINCIPAL INVESTIGATOR: Dr. Sandor L. Lehoczky

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Szofran, F.
Gillies, D.NASA Marshall Space Flight Center (MSFC)
NASA Marshall Space Flight Center (MSFC)

Task Objective:

The major objective of this research is to establish the limitations imposed by gravity during growth on the quality of bulk solid solution crystals having large separation between their liquidus and solidus temperatures. The important goal is to explore the possible advantages of growth in the absence of gravity.

Task Description:

The alloy system being investigated is $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ with x -values appropriate for infrared detector applications in the 8 to 14 μm region. Both melt and Te-solvent growth methods as well as growth in magnetic fields are being considered. The study consists of flight experimentation and ground-based experimental and theoretical work needed to establish material properties and optimum experimental parameters for the on-going flight experiment and to assist material evaluation. $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ is representative of several alloys which have electrical and optical properties that can be compositionally tuned to meet a wide range of technological applications in the areas of sensors and lasers with applications to optical computing and communications as well as the national defense. The investigation includes both Bridgman-Stockbarger and solvent growth methods, as well as growth in a magnetic field. The alloys are prepared by reacting pure, elemental constituents in evacuated, sealed, fused-silica ampoules. The crystals are grown in a multizone furnace. The hot zone is heated above the liquidus temperature of the given alloy and the cold zone is maintained at lower temperatures to provide a temperature gradient sufficient to prevent constitutional supercooling. Crystal growth is accomplished by slowly moving the ampoule from the hot zone to the cold zone of the furnace.

The majority of the ground-based studies are being performed in the Space Sciences Laboratory of the George C. Marshall Space Flight Center. The flight portion of the investigation is being conducted using the Advanced Automatic Directional Solidification Furnace developed by the Marshall Space Flight Center and manifested for flights on the United States Microgravity Payload series of missions. The first flight of the instrument took place in March 1994.

Task Significance:

The anticipated results of this study will have both scientific and technological significance. The advancement in science will result from the increased understanding of the role of gravity on the fluid dynamic and compositional redistribution phenomena during the crystal growth of solid-solution semiconducting alloys having large separation between the liquidus and solidus of the constitutional phase diagrams, and from the more accurate values of materials properties that can be measured using the high-quality, bulk crystals grown in space. Any advance in quality of these electronic materials has a great technological impact because of the application to infrared detectors for NASA and DoD requirements.

Progress During FY 1996:

Characterization continued on the boule grown during the USMP-2 Mission. The work included extensive compositional determination using in-house energy dispersive (EDS) and wavelength dispersive x-ray analysis (WDS) and WDS performed at Princeton Research Institute. These data demonstrated conclusively the effects of fluid flow on solid solution crystal growth at low acceleration levels. Of particular significance was the dramatic differences observed with different attitudes of the space shuttle and resultant different steady acceleration components.

The experimental data gathered from USMP-2 is being used to define the acceleration requirements needed for USMP-4, and the optimum directions and values of the resultants. Such requests have been transmitted to the

Mission teams and incorporated into the USMP-4 time line. Due to time constraints on USMP-4, the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ crystal to be grown will be pre-processed so that the liquid boundary layer will exist in the sample and will be retained during directional back melting on orbit. Unlike the USMP-2 experiment, the sample will be seeded with a cadmium telluride <111> oriented crystal. At this stage, two samples are being prepared, one with $x = 0.152$, which is the primary and one with $x = 0.200$ which is the back up.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	3
MS Students:	2	MS Degrees:	5
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 10/84 EXPIRATION: 10/98

PROJECT IDENTIFICATION: 963-35-01

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Gillies, D.C., Lehoczky, S.L., Szofran, F.R., Watring, D.A., and Alexander, H.A. Effects of Residual Accelerations during Microgravity Directional Solidification of Mercury Cadmium Telluride on the USMP-2 Mission. *J. Crys. Growth* (in press).

Li, W., and Patterson, D. Electronic and Formation Energies for Deep Defects in Narrow-Gap Semiconductors. *Phys. Rev B*, vol. 53, 15622-15630 (1996).

Watring, D.A., and Lehoczky, S.L. Magneto Hydrodynamic Damping of Convection during Vertical Bridgman-Stockbarger Growth of HgCdTe . *J. Crys. Growth*, vol. 164, 478-487 (1996).

Proceedings

Bune, A.V., Gillies, D.C., and Lehoczky, S.L. "Evaluation of Temperature Gradient in Advanced Automated Directional Solidification Furnace (AADSf) by Numerical Simulation." *Proceedings of SPIE - The International Society for Optical Engineering - 1996 International Symposium on Space Processing of Materials*, Denver, Colorado, August 4-6, 1996, vol. 2809, 196-204 (1996).

Bune, A.V., Gillies, D.C., and Lehoczky, S.L. "Optimization of Bulk HgCdTe Growth in a Directional Solidification Furnace by Numerical Simulation." *Mat. Res. Soc. Symp. Proceedings*, vol. 398, 139-144 (1996).

Gillies, D.C., Reeves, F.A., Jeter, L.B., Sledd, J.D., Cole, J.M., and Lehoczky, S.L. "The Advanced Automatic Directional Solidification Furnace." *Proceedings of SPIE - The International Society for Optical Engineering - 1996 International Symposium on Space Processing of Materials*, Denver, Colorado, August 4-6, 1996, vol. 2809, 329-335 (1996).

Lehoczky, S.L., Szofran, F.R., and Gillies, D.C. "Growth of Solid Solution Single Crystals." *Second United States Microgravity Payload: One Year Report*, P.A. Curreri and D.E. McCauley, eds., NASA Technical Memorandum 4737, 90-134 (1996).

Lehoczky, S.L., Szofran, F.R., Gillies, D.C., and Watring, D.A. "Growth of Solid Solution Single Crystals." *Proceedings of the 1996 Microgravity Materials Science Conference*, Huntsville, Alabama, June 10-11, 1996 (in press).

Volz, M.P., Szofran, F.R., Watring, D.A., Gillies, D.C., Su, C.-H., and Lehoczky, S.L. "Magnetic Damping of Convective Flows During Semiconductor Crystal Growth." *Proceedings of the International Workshop on High Magnetic Fields*, Tallahassee, Florida, February 28 - March 1, 1996 (in press).

Watring, D.A., Lehoczky, S.L., Szofran, F.R., and Gillies, D.C. "Convection Influence on Radial Segregation During Unidirectional Solidification of the Binary Alloy, HgCdTe ." *Proceedings of SPIE - The International Society for Optical Engineering - 1996 International Symposium on Space Processing of Materials*, Denver, Colorado, August 4-6, 1996, vol. 2809, 57-68 (1996).

Presentations

Bune, A.V., Gillies, D.C., Watring, D.A., and Lehoczky, S.L. "Modeling of Convection and Segregation During HgCdTe Directional Solidification with Emphasis on Coupling with Crystal-Melt Interface Alteration." *Tenth American Conference on Crystal Growth*, Vail, Colorado, August 4-9, 1996.

Gillies, D.C., Lehoczky, S.L., Szofran, F.R., Watring, D.A., and Alexander, H.A. "Effect of Residual Acceleration during Microgravity Directional Solidification of Mercury Cadmium Telluride on the USMP-2 Mission." *Tenth American Conference on Crystal Growth*, Vail, Colorado, August 4-9, 1996.

The Study of Dopant Segregation Behavior During the Growth of GaAs in Microgravity

PRINCIPAL INVESTIGATOR: Prof. David H. Matthiesen

Case Western Reserve University

CO-INVESTIGATORS:

Kaforey, M.
Chait, A.
Kafalas, J.
Carlsan, D.

Case Western Reserve University (CWRU)
NASA Lewis Research Center (LeRC)
Viable Systems, Inc.
M/A Com Associates

Task Objective:

To design, fabricate, process, and analyze selenium-doped gallium arsenide (Se/GaAs) crystals grown in the Crystal Growth Furnace (CGF) on the ground and during the Second United States Microgravity Laboratory mission (USML-2). Specifically, to investigate techniques for obtaining complete axial and radial dopant uniformity during crystal growth of Se/GaAs, and to characterize and, if possible, controllably modify the melt-solid interface shape during the growth of Se/GaAs to achieve uniform radial segregation of the dopant.

Task Description:

Selenium doped gallium arsenide crystals were grown in the CGF during ground-based experimentation and on board USML-2. Characterization of these crystals will include optical (infrared transmission, Fourier Transform Infrared Spectroscopy (FTIR), and Quantitative Infrared Imaging (QIR)), electrical (Hall effect, Capacitance-Voltage (C-V), spreading resistance, and Deep Level Transient Spectroscopy (DLTS)), and chemical (Secondary Ion Mass Spectroscopy (SIMS)) analysis. Experimental results will be compared with theoretical predictions.

Task Significance:

The Current Pulse Interface Demarcation (CPID) system on the CGF will be used to demark the melt-solid interface. These demarcation lines will show the interface shape and location at specific times during solidification. This should lead to an improved understanding of the axial and radial segregation contributions to the concentration distribution.

Progress During FY 1996:

Two selenium doped gallium arsenide crystals were grown in the Crystal Growth Furnace (CGF) on the Second United States Microgravity Laboratory (USML-2). Ground-based experimentation was completed including the growth of two ground truth samples for comparison with the flight samples. Characterization of all of these samples is in progress.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 2
MS Students: 1
PhD Students: 0

TASK INITIATION: 5/92 EXPIRATION: 12/97
PROJECT IDENTIFICATION: 963-35-05
NASA CONTRACT NO.: NAS8-397
RESPONSIBLE CENTER: MSFC

GaAs Crystal Growth Experiment

PRINCIPAL INVESTIGATOR: Prof. David H. Matthiesen

Case Western Reserve University

CO-INVESTIGATORS:

Kafalas, J.A.

Ditchek, B.M.

GTE Laboratories, Inc. (retired)

GTE Laboratories, Inc.

Task Objective:

The objective is to determine the magnitude of effects of buoyancy-driven convection on the crystal growth of bulk gallium arsenide (GaAs).

Task Description:

Selenium-doped ($\sim 10^{-17}$) GaAs crystals are grown in controlled environments at selected environments affecting fluid flow as follows: (a) low-gravity (minimal convection), and (b) normal gravity in three separate orientations (vector stabilizing the temperature gradients, vector destabilizing the thermal gradient, and vector transverse to the thermal gradient), and a magnetically damped flow (the three normal-gravity orientations with either axial or radial magnetic field). The distribution of dopant is measured and compared to numerical predictions. Selected electrical and chemical properties are measured and correlated with the dopant distribution. Both macro- and micro-segregation are determined.

Task Significance:

Gallium arsenide (GaAs), an electronic material, has two principle advantages over silicon for producing solid state electronic "chip:" its ability to emit light, useful for making lasers, and its inherently high speed, useful in high-speed computers, communication satellites, etc. To fully exploit these characteristics, the material must be of the highest quality and be uniformly doped with traces of impurities. Typically, such uniformity is determined by convection in the molten material from which GaAs crystals are grown.

This materials processing experiment, part of a larger effort to better understand and control the crystal growth process, was undertaken to investigate the effects of buoyancy-driven convection on crystal growth.

Progress During FY 1996:

During late 1994 and 1995, an advanced Ph.D. candidate (Mr. Eugene Garza) was provided access to the flight samples in order to complete the secondary ion mass spectroscopy (SIMS) measurements of selenium distribution. He implemented improved techniques for these quantitative measurements on advanced mass spectrometers at the University of Illinois and at the Wright Patterson Materials Laboratory. The measurements were completed and the results summarized as part of Garza's thesis (thesis submitted in FY95 and degree to be granted in FY97). These results and correlated analyses of thermal and fluid transport (due to A. Chait at LeRC) will be summarized in the project final report.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	2	BS Degrees:	1
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	0

TASK INITIATION: 9/85 EXPIRATION: 1/97

PROJECT IDENTIFICATION: 963-21-05-02

NASA CONTRACT NO.: NAG3-147

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Yao, M.W., Matthiesen, D.H., and Chait, A. Numerical simulation of heat transport and fluid flow in directional crystal growth of GaAs. Numerical heat Transfer, Part A: Applications, (accepted, 1996).

Diffusion Processes in Molten Semiconductors

PRINCIPAL INVESTIGATOR: Prof. David H. Matthiesen

Case Western Reserve University

CO-INVESTIGATORS:

Arnold, W.
Chait, A.
Stroud, D.

Case Western Reserve University
NASA Lewis Research Center (LeRC)
Ohio State University

Task Objective:

For FY1996, DPIMS is concentrating on Phase I, which is a flight of opportunity on MSL-1 (STS-83) in March 1997. The Phase I objectives are to provide purely diffusive experimental measurements of the isothermal diffusion coefficients of Ga, Sb and Ga/Si Sb in molten germanium with sufficient accuracy and precision to:

- a) Differentiate between model predictions of the temperature dependence.
- b) Determine the effect of dopant size and type.
- c) Determine if a "wall effect" is present.
- d) Provide input to continuum and atomistic model development.
- e) Provide a preliminary evaluation of dopant-dopant interactions.

To develop a 2-dimensional, fully time dependent continuum numerical model of the germanium diffusion column, shear cell, cartridge and furnace for both earth-based and space-based experiments which accurately predicts the measured concentration profile as a function of distance in the diffusion column.

To develop atomistic models which accurately predict:

- a) The purely diffusive isothermal diffusion coefficient of a dopant in a molten semiconductor,
- b) The temperature dependency of dopants in molten semiconductors, and which:
- c) Attempts to explain the "wall effect,"
- d) Develops new empirical potentials useful for predicting other diffusion and transport properties for other molten semiconductor systems.

Task Description:

This program of study is directed at the fundamental and applied issues pertaining to diffusion of species in the liquid state as driven by concentration gradients (Fickian diffusion) and thermal gradients (Soret diffusion). The fundamental material systems of interest for near term study are the dilute binary systems of gallium (Ga), antimony (Sb) and a dilute ternary system of gallium and silicon in germanium (Ge). Systems of commercial interest for future study include the binary systems of germanium and silicon. This research program consists of three major components: an experimental measurement portion, a continuum numerical simulation portion and an atomistic numerical simulation portion.

The experimental measurement portion is designed to provide definitive measurements of the purely diffusive component of mass transfer in molten semiconductor systems. A shear cell technique will be used to directly measure the diffusion coefficients in semiconductor melts. For the Fickian diffusion case, isothermal measurements will be used to determine the diffusion coefficients. An experimental matrix will be used to determine the dependence of the diffusion coefficients on temperature, dopant type and column diameter. For the Soret diffusion case, measurements will be made in a thermal gradient.

Task Significance:

The fundamental mechanisms of mass diffusion in the liquid state are still unclear to the degree necessary for the prediction of diffusion of one species into another or even within itself. This observation is especially true with respect to the dependency of diffusion mechanisms on temperature and on concentration levels, as well as on the dopant type. Present estimates of diffusivity in molten semiconductors can typically provide an order of magnitude estimate only, without any information on their dependency on concentration levels and types, and on temperature and temperature gradients.

The availability of these data is of paramount importance for practical reasons as well. The relevancy of numerical modeling for the analysis and design of ground based and space experiments is directly dependent upon the accuracy of the fundamental material properties used in these simulations. These data are also important for the correct characterization and interpretation of experimental results from ground based and space experiments.

The subject of how a mass of one species diffuses through a matrix of another is, at the same time, both a very old and very new research area. That this area can encompass the small, i.e., movement of electrons in a plasma, to the very large, i.e., the depletion of the global ozone layer, merely serves to emphasize the fundamental aspects of this subject. Most manufacturing technologies at some stage, rely on diffusion processes in the solid, liquid or gas.

The need for precise measurements of the diffusion coefficients in molten semiconductors has been repeatedly pointed out. These data are required both to interpret the experimental results from previous space-based (and Earth-based) experiments and also to optimize newly envisioned experiments. Difficulties in experimental techniques and theoretical interpretations are cited for the lack of these data. This is a comprehensive program which addresses both of these issues.

Progress During FY 1996:

Experiments:

- Have made several measurements of the diffusion coefficient of Ga in Ge at 960°C, 1000°C and 1550°C in both 1.5 mm and 3mm capillaries.
- Have made measurements of the diffusion coefficient of Sb in Ge at 1000°C in both 1.5 mm and 3.0 mm capillaries.
- Final experimental procedures for MSL-1 were approved.

Engineering:

- Design modifications were made to insure that no interface movement of the diffusion couple will occur during alignment.

Science:

- Interface movement was numerically modeled and found to strongly affect the measured diffusion coefficient.
- Chemical measurements of the concentration profile at several diffusion experiments were compared with mass considerations to determine interface movement in past experiments.
- Final flight dopants were determined for MSL-1.
- Final SRD submitted to HDQ.
- Developed a Soret "check" to determine the influence at small unmeasurable temperature gradients on the measured diffusion coefficient.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	2	MS Degrees:	1
PhD Students:	0	PhD Degrees:	0

TASK INITIATION: 1/93 EXPIRATION: 2/97

PROJECT IDENTIFICATION: 963-21-05-04

NASA CONTRACT No.: NCC3-293

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Arnold, W., Matthiesen, D., Bennett, R., and Jayne, D., An innovative method for preparing semiconductor charges used in crystal growth and shear cell diffusion experiments. J. of Crystal Growth, (accepted 1996).

Space- and Ground-Based Crystal Growth using Magnetically Coupled Baffle

PRINCIPAL INVESTIGATOR: Dr. Aleksandar G. Ostrogorsky

Rensselaer Polytechnic Institute

CO-INVESTIGATORS:

Duffar, T.

Centre d'Etudes Nucleaires (Grenoble, France)

Task Objective:

The main objective is to develop a method for crystal growth which is less sensitive to residual acceleration than the conventional methods (Bridgman and zone freezing). This method will be used to demonstrate that in space laboratories, important semiconductor crystals can be grown under the ideal steady-state conditions, resulting from diffusion controlled solidification. We plan to use a magnetically suspended baffle (i) to reduce the characteristic size of the melt, and make it less sensitive to longitudinal and lateral acceleration and (ii) premix the melt and expect to obtain semiconductors of exceptional crystalline and chemical perfection. Furthermore, the segregation data obtained in microgravity will be used to test the non-dimensional parameter named the Segregation number (developed under previous NASA sponsorship), which can be used to select dopants and growth parameters for space experiments.

Task Description:

Different design options for retaining and driving the baffle by magnetic coupling to a high Curie temperature alloy slug will be considered and tested. The transparent two zone vertical Bridgman furnace will be modified and used for ground-based studies. Doped GaSb and Ge crystals will be grown using directional and zone solidification methods. Current pulsing will be used to mark the solid-liquid interface (Peltier marking). The position of the interface will be determined by measuring the electrical resistance of the sample, which changes due to the change in the solid/liquid fraction. The spectral element code NEKTON will be used to conduct parametric studies, in order to optimize the crystal growth process both on earth and in microgravity. It is proposed that two ampoules with doped GaSb (one with the baffle and one without the baffle, for comparison) are solidified in microgravity. The effect of convection on segregation and formation of dislocations and twins will be studied.

Task Significance:

The baffle controlled by magnetic coupling should (at a minute expense in space and weight) provide the two key features that are impeding the quality of space-grown crystals: (i) homogeneous starting melt, and (ii) the addition melt stabilization needed to switch from weak mixing to insignificant mixing (i.e., convection-free growth). This will bring the properties of the space-grown crystals closer to the theoretical predictions (all models use assumption of homogeneous starting melt) and to the theoretical limits of compositional and crystalline perfection. The ground-based and flight studies will advance our understanding of segregation and formation of crystalline imperfections.

Progress During FY 1996:

The thrust during the first three months of this project (the project started in July 1996) was directed at consolidation of the experimental basis for crystal growth and characterization. The multizone Mellen furnace was serviced, upgraded and calibrated. The precision ID diamond saw (the thickness of the saw blade is 0.2 mm) was reconditioned and connected to a computer. A programmable power supply capable of producing electrical current pulses of controlled amplitude (up to 100 A) and duration (up to 100 msec) is under construction. This setup will be used for Peltier marking of the interface position and shape in 32 mm diameter GaSb and Ge crystals. Since transients in the initial growth rate are unavoidable, we are developing an analytical model of diffusion-controlled segregation which allows for transient growth rates (the Tiller's model considers only a constant solidification rate). This model will be used for analyzing the initial transient in solute distribution of space-grown crystals.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NCC8-97

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Ostrogorsky, A.G. "Space- and Ground-Based Crystal Growth Using a Magnetically Coupled Baffle." Microgravity Materials Science Conference, Von Braun Civic Center, Huntsville, Alabama, June 10-11, 1996, pp 138-139.

*Comparison of Structure and Segregation in Alloys Directionally Solidified in Terrestrial and Microgravity Environments***PRINCIPAL INVESTIGATOR:** Prof. David R. Poirier

University of Arizona

CO-INVESTIGATORS:Heinrich, J.C.
Tewari, S.N.University of Arizona
Cleveland State University**Task Objective:**

This is a program to conduct experiments in a long duration microgravity environment, with the objective of studying dendritic microstructures and segregation in directionally solidified dendritic alloys. The research builds on our previous grant in which we generated an extensive data base on directionally solidified Pb-Sn alloys and simulated solidification of the alloys using continuum theory of porous media. Based on our previous research, it is clear that thermosolutal convection masks the effects of diffusional transport during solidification and also leads to macrosegregates known as freckles. We are convinced, therefore, that with terrestrial experiments, diffusive and convective phenomena occur simultaneously, which complicate the study of dendritic growth. In microgravity, however, it would be possible to effect directional solidification with no thermosolutal convection. Our hypotheses are the convection and attendant macrosegregation will be eliminated and the dendritic microstructure will be greatly altered in microgravity.

Task Description:

The PI and one of the co-investigators met with a team of engineers and scientists at MSFC to see the High Gradient Fast Quench Furnace (HGFQ) and to plan the collaborative research between the universities involved, MSFC, and LeRC. Directional solidification experiments on a Pb-Sn alloy and on a Al-Cu alloy have been outlined, using different growth conditions to effect different dendritic microstructures. Numerical modeling to simulate the transport phenomena and solidification in the planned experiments is currently underway at MSFC and the University of Arizona. Preliminary experiments related to capsule materials are underway at Cleveland State University. As ingot-samples are prepared at MSFC, they will be characterized for dendrite morphology, macrosegregation and possibly microsegregation.

Task Significance:

Models of dendritic solidification that are used to predict the undercooling during growth of alloys rely on the assumption of diffusional transports of both heat and solute. An important feature of the models is a prediction of the dendrite tip radius. However, the thermosolutal convection of liquid in, from, or close to the solid plus liquid region of solidifying alloys masks the diffusional processes at the dendrite tips and is responsible for most macrosegregation in castings and ingots. Availability of microgravity provides an opportunity to obtain experimental data, where thermosolutal convection is negligible. With the new grant, growth conditions for such microgravity experiments will be defined by combining mathematical modeling and simulations with the results of terrestrial experiments. Thermosolutal convection will be significantly reduced in microgravity, and thus we can compare segregation and microstructure in specimens terrestrially solidified and those solidified in microgravity.

In terrestrial experiments, dendritic solidification is difficult to study because specimens are plagued with severe forms of macrosegregation caused by thermosolutal convection, including: 1) continuous segregation from end-to-end; 2) occurrence of localized segregates referred to freckles; and, 3) dendrite clustering. In the microgravity environment, the thermosolutal convection will be greatly diminished, and the convection will be confined mainly to the minor flows of interdendritic liquid required to satisfy solidification shrinkage and possibly due to "g-jitter." Morphological features, metrics, and segregation in samples directionally solidified in an earth-based furnace and in samples grown in microgravity are expected to be quite different.

Progress During FY 1996:

Since the grant only started on June 1, 1996, we have no progress to report as of this writing.

II. MSAD Program Tasks — Flight Research

Discipline: Materials Science

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 1

PhD Students: 0

TASK INITIATION: 6/96 EXPIRATION: 5/99

PROJECT IDENTIFICATION:

NASA CONTRACT No.: NCC8-96

RESPONSIBLE CENTER: MSFC

Temperature Dependence of Diffusivities in Liquid Metals

PRINCIPAL INVESTIGATOR: Prof. Franz E. Rosenberger

University of Alabama, Huntsville

CO-INVESTIGATORS:

Banish, R.M.

University of Alabama at Huntsville (UAH)

Task Objective:

This research aims at advancing the understanding of diffusion mechanisms in liquid metals and alloys through accurate diffusivity measurements over a wide range of temperatures, including the proximity to the materials' melting points.

Task Description:

Toward the task objective we are pursuing the following tasks:

- Development of an efficient technique for dynamic *in situ* measurements of diffusivities in melts as a function of temperature;
- Development of a flight-certified hardware package to automatically perform such diffusivity measurements under reduced gravity conditions and on Earth;
- Investigation of the significance of the "wall effect" in diffusion capillaries;
- Exploration of convective contamination of the diffusivity measurements on Earth through numerical modeling; and,
- Measurements of diffusivities of selected materials that will be chosen according to class-like molecular interaction behavior in the liquid.

Diffusivities will be determined from temporal records of evolving concentration profiles through multi-detector measurements of radioactive tracer emission. An initially solid, cylindrical sample contains a radioactive isotope at one end. After melting, radiation escaping through small bores in an isothermal liner/radiation shield is monitored via a chain of detectors. Data evaluation is facilitated by a novel algorithm, which is not limited to the simple initial conditions traditionally used in diffusivity studies. The algorithm permits data deduction from any sequence of concentration distributions. Hence, diffusivity data can be gathered over a range of temperatures in a single experiment. Utilizing the different radiation absorption behavior of different photon energies, we will investigate the significance of the "wall" effect. This effect is currently believed to contaminate diffusion studies in narrow capillaries used to suppress convection at normal gravity.

Task Significance:

The diffusion of species in melts and its temperature dependence is important for product quality in numerous metallurgical and semiconductor manufacturing processes. Hence, a detailed understanding of diffusion in liquid metals and alloys is essential for an efficient improvement of numerous technological processes. Neither accurate measurements nor reliable theories of diffusion in liquids are available at this point. The uncertainties in the experimental values are due to difficult-to-control transport contributions from convection. The complex structure of liquids has resulted in an abundance of theoretical models of liquid diffusion. This investigation will provide accurate data for selected materials over wide temperature ranges that can be used for both process development and verification of theoretical models.

Progress During FY 1996:

- Construction and flight-certification (U.S. and Russian) of a low temperature (185 °C) version of our liquid metal diffusion experiment in response to an immediate flight opportunity utilizing the Microgravity Isolation Mount (MIM) aboard Mir. Measurements to be conducted under both defined acceleration inputs and vibration isolation will provide data for comparison with our numerical modeling efforts and guidance for the later high temperature experiments.
- Development of solid state diffusion bonding between radioactive and nonradioactive sample sections, and of spring-loading the whole diffusion sample. These measures will mitigate the formation of voids and bubbles during the liquid diffusion experiment.

- Verification of various experiment design assumptions through tracer diffusion experiments in both solid and liquid samples.
- Minimization of the radioisotope concentration (activity) through optimization of the sample view factor and signal-to-noise-ratio obtained in a sequence of measurements at different sample activities.
- Design and construction of combined dual detector-preamplifier-discriminator units to minimize components and improve the electronic shielding.
- Numerical modeling of the time-dependent and three-dimensional diffusive-convective transport in typical experiment geometries with realistic boundary conditions. In particular, the results show that the magnetic field strengths required to assure dominantly diffusive transport at unit gravity are so high that the diffusivity itself would be modified.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 2/93 EXPIRATION: 5/98

PROJECT IDENTIFICATION: 963-35-21

NASA CONTRACT No.: NAS8-397

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Banish, R.M., Alexander, J.I.D., Jalbert, L.B., and Rosenberger, F. "*In situ* radiotracer diffusion measurement technique (invited paper)." Gravitational Effects in Fluid and Materials Science Commission Meeting, 31st COSPAR Scientific Assembly, Birmingham, England, July 1996.

Banish, R.M., Jalbert, L.B., Roberson, R.J., and Rosenberger, F. "*In situ* radiotracer diffusion measurement technique (invited paper)." Space Processing of Materials Symposium, 1996 SPIE, Denver, Colorado, August 1996.

Self-Diffusion in Liquid Elements

PRINCIPAL INVESTIGATOR: Prof. Franz E. Rosenberger

University of Alabama, Huntsville

CO-INVESTIGATORS:

Banish, R.M.

University of Alabama at Huntsville (UAH)

Task Objective:

This research aims at advancing the understanding of self-diffusion mechanisms in liquids through accurate diffusivity measurements over a wide range of temperatures, including the proximity of the elements' melting points.

Task Description:

Toward the task objective we are pursuing the following tasks:

- Development of an efficient technique for dynamic *in situ* measurements of diffusivities in melts as a function of temperature;
- Development of a flight-certified hardware package to semi-automatically perform such diffusivity measurements under reduced gravity conditions and on Earth;
- Investigation of the significance of the "wall effect" in diffusion capillaries, which is currently believed to contaminate diffusion studies in narrow capillaries used to suppress convection at normal gravity;
- Exploration of convective contamination of the diffusivity measurements on Earth through numerical modeling; and,
- Measurements of diffusivities of selected elements that will be chosen according to class-like molecular interaction behavior in their liquid.

Diffusivities will be determined from temporal records of evolving concentration profiles through multi-detector measurements of radioactive tracer emission. An initially solid, cylindrical sample contains a radioactive isotope at one end. After melting, radiation escaping through small bores in an isothermal liner/radiation shield is monitored via solid-state detectors. Data evaluation is facilitated by an algorithm, which is not limited to the simple initial conditions traditionally used in diffusivity studies. The algorithm permits data deduction from any sequence of concentration distributions. Hence, diffusivity data can be gathered over a range of temperatures in a single experiment. Utilizing the different radiation absorption behavior of different photon energies, we will investigate the significance of the "wall" effect.

Task Significance:

The diffusion of species in liquids and its temperature dependence is important for both fundamental reasons and the optimization of numerous manufacturing processes. Neither accurate measurements nor reliable theories of diffusion in liquids are available at this point. The complex structure of liquids has resulted in an abundance of theoretical models of liquid diffusion. The uncertainties in the experimental values are due to difficult-to-control transport contributions from convection. This investigation will provide accurate data for selected simple liquids (molten elements) over wide temperature ranges for the verification of theoretical models.

Progress During FY 1996:

- Design of a high temperature (900 °C) prototype hardware for diffusivity measurements at multiple temperatures.
- Numerical optimization of the radiation port locations allowing for diffusivity measurements at multiple temperatures in one sample. This model accounts for the thermal expansion properties of the sample containment and positioning components, and the thermally induced position changes of the radiation ports.
- Construction and thermal testing of the prototype hardware.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 **EXPIRATION:** 11/99

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NCC8-99

RESPONSIBLE CENTER: MSFC

Particle Engulfment and Pushing by Solidifying Interfaces

PRINCIPAL INVESTIGATOR: Dr. Doru M. Stefanescu

University of Alabama, Tuscaloosa

CO-INVESTIGATORS:

Curreri, P.A.
Dhindaw, B.K.
Sen, S.
Juretzko, F.R.
Bhamidipati, R.

NASA Marshall Space Flight Center (MSFC)
I.I.T. (Kharagpur, India)
Universities Space Research Association/MSFC (USRA)
University of Alabama
University of Alabama

Task Objective:

The primary objective of this task is to further develop the existing understanding on pushing and engulfment of particles by planar liquid/solid interfaces during solidification of metallic alloys.

The approach towards achieving this objective is by developing an analytical and then numerical model describing the phenomenon, with a parallel experimental validation effort. The numerical model is required in order to include the effect of convection in the liquid on interface morphology and the particle/interface interaction. The interaction between an insoluble ceramic particle and a liquid-solid interface during solidification is significantly influenced by gravitational acceleration. Since the interaction between an insoluble ceramic particle and a liquid-solid interface during solidification is significantly influenced by gravitational acceleration, microgravity experiments will be performed to validate these models and to further contribute to the experimental data base for metals/ceramic particulate mixtures.

Task Description:

To acquire further insight in the physics of particle behavior, directional solidification experiments with transparent organic materials doped with polystyrene particles were also scheduled. It was planned to use results from these experiments to validate the analytical model developed so far.

Ground-based experiments under controlled solidification conditions with Al-SiC and Al-ZrO₂ systems to document pushing/engulfment phenomena in metallic systems were also scheduled. In addition several tasks required in the flight requirements definition effort were to be performed.

In addition to the original tasks, the LMS mission scheduled for flight in summer 1996 created the opportunity for some early (unscheduled) flight experimentation. Ground experiments were used to outline the processing parameters. Sample cartridges had to be designed and then tested with thermal models for compatibility with the sample design. In a parallel effort it was necessary to produce suitable samples for the flight experiment.

Task Significance:

It is of fundamental and practical importance to understand and control particle behavior at the solid/liquid interface during solidification. Particle behavior determines the uniformity of their distribution in the matrix. Uniformity of particle distribution is of great significance as it dictates the mechanical and physical properties of the composites.

Introduction of insoluble ceramic particles in a metal matrix primarily involves three stages: transfer of particles from gas to liquid, interaction of particles in the liquid state, and finally, transfer of particles from liquid to solid. It is the last stage that is the most important and yet the least understood since it is the outcome of the interaction of numerous solidification variables. The anticipated results from this research program will provide a much better understanding of this stage of metal matrix composites processing and therein lies its significance.

Progress During FY 1996:

During FY96 the work on the analytical model was continued which led to modifications of the model. The use of the thermal conductivity ratio in the governing equation was modified, an exact calculation of the exponent used in the definition of the repulsive force based on surface energy was provided, and a new value for the minimum particle

interface distance was proposed. A methodology was developed to calculate the parameter Δg , which determines the repulsive force acting on the particle. This methodology was applied to the current systems under investigation. The comparison with experimental results yielded a reasonable correlation.

Work on the evaluation of the critical velocity was continued in the aluminum/zirconia system. This work included the use of smaller particles (200 μm dia.) in addition to the previously used size of 500 μm dia. The ground experiments yielded a well defined transition velocity for the model system aluminum/zirconia. Evaluation of the critical velocity of metallic model systems was extended to the zinc/zirconia system where the ratio of melt and particle density is reversed. As in the initial Al/ZrO₂ system, a critical velocity could be established for the Zn/ZrO₂ system. In aluminum-nickel eutectic system such a particle engulfment transition could not be unambiguously determined.

Two pure aluminum samples containing zirconia particles, and one sample with an aluminum/nickel matrix of eutectic composition with zirconia particles, were selected as flight samples. These samples were characterized using the newly developed x-ray transmission microscope, located at MSFC, for sample integrity and suitable particle distribution. Further ground tests were performed to optimize the sample design.

These samples were flown during the LMS mission (STS-78). The temperature profile was constantly monitored during the experiments. All three experiments performed nominally. Preliminary x-ray investigation of the samples showed that the sample designs were correct and the cartridge performance was as expected.

Work on transparent model substances was focused on further purification of the selected substances, namely succinonitrile and biphenyl. This purified matrix material will be used for the samples of an upcoming glovebox experiment in the summer of 1997. The design and assembly of the hardware was continued as was the design and prototype production of flight samples.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 2
PhD Students: 1

TASK INITIATION: 2/93 EXPIRATION: 7/97
PROJECT IDENTIFICATION: 963-35-22
NASA CONTRACT No.: NAS8-397
RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Curreri, P.A., and Kauckler, W.F. Real-time x-ray transmission microscopy of solidifying Al-In alloys. *Met. Trans.*, vol. 27A, 801-808 (1996).

Sen, S., Dhindaw, B.K., Stefanescu, D.M., Catalina, A., and Curreri, P.A. Melt convection effects on the critical velocity of particle engulfment. *J. of Crystal Growth*, (accepted, 1996).

Proceedings

Dhindaw, B.K., Ganguly, P., Juretzko, F.R., and Stefanescu, D.M. "Particle redistribution during remelting of Al/SiCp composites - an experimental and computational study." Annual TMS meeting and exhibition, R. Schiffman, ed., Anaheim, California, February 1996.

Juretzko, F.R., Dhindaw, B.K., Sen, S., and Stefanescu, D.M. "The use of x-ray transmission microscopy in the evaluation of particle distribution in metal ceramic composites (extended abstract)." 3rd International Conference on Composite Engineering ICCE/3, p 421, New Orleans, Louisiana, July 1996.

Juretzko, F.R., Stefanescu, D.M., Dhindaw, B.K., and Sen, S. "Interfacial Energy $\Delta\gamma$ - theoretical and experimental evaluation for metal-ceramic systems." ASM-TMS materials week '96, Cincinnati, Ohio, October 1996 (in print).

Presentations

Stefanescu, D.M. "Particle Pushing and Engulfment by Solidifying Interfaces." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Crystal Growth of ZnSe and Related Ternary Compound Semiconductors by Physical Vapor Transport

PRINCIPAL INVESTIGATOR: Dr. Ching-Hua Su

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Brebrick, R.

Volz, M.

Sha, Y.

Noever, D.

Sanghanitra, S.

Johnson, S.

Marquette University

NASA Marshall Space Flight Center (MSFC)

Universities Space Research Association (USRA)

NASA Marshall Space Flight Center (MSFC)

Santa Barbara Research Center

Santa Barbara Research Center

Task Objective:

The investigation consists of extensive ground-based experimental and theoretical research efforts and concurrent flight experimentation. The objectives of the ground-based studies are to obtain the experimental data and conduct the analyses required to define the optimum growth parameters for the flight experiments, perfect various characterization techniques to establish the standard procedure for material characterization and quantitatively establish the characteristics of the crystals grown on Earth as a basis for subsequent comparative evaluations of the crystals grown in a low-gravity environment, and develop theoretical and analytical methods required for such evaluations.

Task Description:

The crystal growth experiment will use a novel vapor transport three-thermal-zone heater translating method. The Crystal Growth Furnace (CGF) or Advanced Automated Directional Solidification Furnace (AADSf) will be ideal for this experiment because they provide two high-temperature end zones and a booster heater at the center of the furnace with translation capability. Using this technique, large single crystals of CdS, CdTe, PbSe, ZnTe, ZnSe, ZnSeTe, and ZnSeS have been grown successfully in this laboratory.

Task Significance:

The materials to be investigated are ZnSe and related ternary semiconducting alloys, e.g., $\text{ZnS}_x\text{Se}_{1-x}$, $\text{ZnSe}_{1-x}\text{Te}_x$, and $\text{Zn}_{1-x}\text{Cd}_x\text{Se}$. These materials are useful for opto-electronic applications such as highly efficient light emitting diodes and low power threshold and high temperature lasers in the blue-green region of the visible spectrum. The recent demonstration of its optical bistable properties also makes ZnSe a possible candidate material for digital optical computers. Compositional non-uniformity, microstructural crystal defects (e.g., dislocations, small-angle grain boundaries, and second phase precipitates), and deviation from stoichiometry can seriously limit state-of-the-art device performance and future device applications. The reduction of gravity-driven convective fluid flows in a low-gravity environment is expected to be advantageous in minimizing these compositional variations and structural defects.

Progress During FY 1996:

1. Mass flux of ZnSeTe and ZnSeS was measured and the results were compared to theoretical calculations.
2. Horizontal and vertical growth of ZnSe, ZnSeTe, and ZnSeS were performed.
3. Seeded growth of ZnSe was conducted.
4. The grown crystals were assessed by characterization methods established earlier.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 2/93 EXPIRATION: 2/96

PROJECT IDENTIFICATION: 963-35-23

NASA CONTRACT NO.: NAS8-397

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Brebrick, R.F., and Fang, R. CdTe II: Defect Chemistry. *J. Phys. Chem. Solids*, vol. 57, 451-460 (1996).

Brebrick, R.F., and Liu, H. Partial Pressures of Zn and Se₂ over ZnSe(s) from Optical Density Measurements. *High Temperature and Materials Science*, vol. 35, 215-237 (1996).

Fang, R., and Brebrick, R.F. CdTe I: Solidus Curve and Composition-Temperature-Tellurium Partial Pressure Data for Te-Rich CdTe(s) from Optical Density Measurements. *J. Phys. Chem. Solids*, vol. 57, 443-450 (1996).

Proceedings

Su, C.-H., Gillies, D.C., Szofran, F.R., Watring, D.A., and Lehoczky, S.L. "The Influence of Reduced Gravity on the Crystal Growth of Electronic Materials." Proceeding of the 6th International Space Conference of Pacific Basin Societies (6th ISCOPS), Marina del Ray, California, "Strengthening Cooperation in the 21st Century, Volume 91, Advances in the Astronautical Sciences" (1996).

Books

Su, C.-H., and Sha, Y.-G. "Current Topics in Crystal Growth Research ("Growth of Wide Band Gap II-VI Compound Semiconductors by Physical Vapor Transport")." Edited by the Council of Scientific Information, Research Trends, vol. 2, pp 401-433, 1995.

Presentations

Sha, Y.-G., Su, C.-H., and Lehoczky, S.L. "Mass Flux of ZnSeS and ZnSeTe by Physical Vapor Transport." MRS Fall Meeting, Boston, Massachusetts, November 27 - December 1, 1995.

Su, C.-H. "Crystal Growth of ZnSe and Related Ternary Compound Semiconductors by Vapor Transport." Microgravity Materials Science Conference, p 176 conference summaries volume, Huntsville, Alabama, June 10-11, 1996.

Su, C.-H., Gillies, D.C., Szofran, F.R., Watring, D.A., and Lehoczky, S.L. "The Influence of Reduced Gravity on the Crystal Growth of Electronic Materials." Invited paper presented at the 6th International Space Conference of Pacific Basin Societies (6th ISCOPS), Marina del Ray, California, December 6 - 8, 1995.

Interface Pattern Selection Criterion for Cellular Structures in Direction Solidification

PRINCIPAL INVESTIGATOR: Dr. Rohit K. Trivedi

Iowa State University

CO-INVESTIGATORS:

Tewari, S.N.

Kurze, D.A.

Cleveland State University

North Dakota State University

Task Objective:

The ability to control microstructures of solidified materials is crucial for obtaining optimum properties of materials processed by casting, welding, or rapid solidification techniques. Since microstructure evolution depends upon processing conditions, the fundamental principles that correlate microstructures with processing conditions must be quantitatively established. Theoretical ideas on microstructure prediction is based on the solution of transport equations which predict multiple solutions, whereas experimental studies show that the system selects a unique solution or a very narrow set of solutions. This research is aimed at establishing the fundamental physics that govern the selection of the unique microstructural features under a given growth condition. The fundamental role of transport and interfacial energy will be quantitatively evaluated through the development of a rigorous quantitative model under diffusion controlled growth, and this model will be tested under a microgravity environment in which convection effects are minimized.

Task Description:

The proposed research will consist of carrying out accurate and rigorous numerical modeling, coupled with critical ground-based and microgravity experimental studies, to quantitatively evaluate the fundamental criterion for the cellular pattern selection.

Initial ground-based studies will be carried out in Al-4 wt% Cu and Al-15 wt % Cu alloys to establish the range of conditions over which cellular structures are stable. The condition for cellular to dendritic transition will also be established. Within the cellular range, the steady state cellular structure will be characterized with respect to the tip temperature, tip composition, cell amplitude, three-dimensional cell shape, and microsegregation patterns. The above characteristics will be examined under different conditions of velocity and temperature gradient. Experiments will also be carried out in Pb-Sn system which requires low furnace temperature. A new design of furnace facility is developed which can allow several samples to be solidified simultaneously under the same growth conditions and under highly controlled thermal conditions.

Since the cellular structures in directional solidification are stable only under low velocity conditions where convection effects are dominant, a systematic study will be carried out in samples of varying diameters, ranging from 200 μm to 1 cm diameter. The change in microstructure with decreasing diameter, which correlates with the decreasing convection effects, will be quantitatively established. For the finer tubes the microstructures will also be influenced by the finite size of the sample, so that the effect of finite sample size will be quantitatively studied. These studies will define conditions for cellular growth in diffusive regime under microgravity conditions.

A detailed mathematical model of cellular growth will be developed to establish the physics of the cellular microstructure selection criterion. An analytical expression will be developed from these results to quantitatively determine the role of various physical processes on the cellular selection criterion. The model will also be analyzed to relate cell tip temperature, cell tip composition, cell amplitude, and microsegregation patterns as a function of velocity. The predictions of the model will then be tested against the benchmark experimental results obtained under microgravity conditions. Besides the physics of the cellular pattern selection, this study will also establish the precise physics which lead to cell-dendrite transition.

Task Significance:

In order to develop optimum properties in the material, a successful processing technique needs to be designed. Since the properties are related to microstructure, the basic concepts that correlate microstructures with processing conditions will be quantitatively identified in this study. The application of the understanding of fundamental physics of microstructural selection criterion obtained in this study will then provide a fundamental theoretical basis to model important industrial processes.

Progress During FY 1996:

A series of experiments have been carried out in Al-4 wt% Cu that was directionally solidified at different velocities. A new experimental technique was developed in which samples of several different diameters can be simultaneously solidified directionally so that the different microstructures could be correlated with the sample diameter. Sample diameters have been varied from 5 mm to 200 μ m. As the sample diameter decreases, the convection effects also decrease. Thus we have been able to quantitatively examine the role of convection on microstructure development. Several new features have been identified. At low velocities, a planar interface is stable in large samples where convection effects are dominant. However, at the same velocity, a cellular structure is observed in thinner tubes. This clearly shows that convection stabilizes the planar interface growth. For a given velocity, the cellular spacing is found to increase, and the cell tip temperature is found to decrease as the diameter of the tube is reduced. A significant effect of convection on cellular microstructure characteristics in larger samples have been identified and quantified, and the minimum diameter of the sample required to suppress convection effect on microstructure formation is established. This critical diameter will be used to obtain a critical Rayleigh number which will allow us to estimate the microgravity level required to minimize convection for the larger diameter samples that will be used in the microgravity study.

A numerical study of cellular growth has been initiated, and the code has been developed to study steady state cellular characteristics. This model will be extended to include diffusion in the solid and to the non-steady state growth conditions.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 422-25-11

NASA CONTRACT No.: NCC8-98

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Trivedi, R., Tewari, S., and Kurtze, D. "Interface Pattern Selection Criterion for Cellular Structures in Directional Solidification." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Coarsening in Solid-Liquid Mixtures

PRINCIPAL INVESTIGATOR: Prof. Peter W. Voorhees

Northwestern University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this project is to plan and perform a microgravity experiment on Ostwald ripening in solid-liquid mixtures. This experiment will serve two primary purposes.

1. It will allow experiments to be performed which can be directly compared to heretofore untested theories for coarsening in systems with low volume fractions of solid.
2. It will eliminate conclusively convection of the liquid matrix and small-scale particle motion within the skeletal structure as possible sources for the disagreement observed between theory and experiment in the high volume fraction experiments.

Task Description:

Previous NASA sponsored work clearly showed that solid-liquid mixtures consisting of Sn-rich particles in a Pb-Sn eutectic liquid are ideal, and perhaps unique, systems in which to explore the dynamics of the Ostwald ripening process. The high coarsening rate in these systems permit accurate kinetic data to be obtained, and the thermophysical parameters necessary to make a comparison between theory and experiment are known. However, in a terrestrial environment experiments can be performed only at the relatively high volume fractions of solid where the presence of a solid skeletal structure prevents large-scale particle sedimentation. In these high volume fraction experiments, a comparison between theory and experiment shows that the solid-liquid mixtures are coarsening faster than predicted by an approximate theory for purely diffusional controlled Ostwald ripening. Thus, we are in the process of formulating a microgravity experiment. This experiment will serve two primary purposes: it will allow experiments to be performed which can be directly compared to heretofore untested theories for coarsening in systems with low volume fractions of solid, and it will eliminate conclusively convection of the liquid matrix and small-scale particle motion within the skeletal structure as possible sources for the disagreement observed between theory and experiment in the high volume fraction experiments.

Task Significance:

The spaceflight experiment will produce data which, for the first time, can be compared directly to theory with no adjustable parameters. This data will address the long standing controversy over the dependence of the coarsening rate of a two-phase system of the volume fraction on coarsening phase.

The results from the spaceflight experiment will further our understanding of the processes responsible for microstructural development in a broad range of commercially important materials ranging from turbine blade alloys to liquid phase sintered materials.

Progress During FY 1996:

Our preparations for the upcoming flight of MSL-1 continue. This past year we completed successfully the Requirements Definition Review. It was decided that the Microgravity Glovebox facility will be used to perform the experiments. We are interacting closely with NASA engineers in the development of a furnace in which to perform the coarsening experiments. We have analyzed the effects of vibrations induced by the glovebox fans on the motion of a solid Sn-rich particle in the Pb-rich liquid. High frequency (60 Hz) vibrations were found to have little influence on the location of the solid particle. In preparation for flight, a furnace has been constructed to grow Sn-bicrystals. These bicrystals will be used to study the temporal evolution of grain boundary grooves in microgravity. The temporal evolution of these grooves will provide information on the thermophysical parameters of the Pb-Sn system. A complete set of samples, that will yield volume fractions of solid of 0.05 to 0.8, has been produced. These samples will be used to test the temperature uniformity, heating rate and cooling rate of the spaceflight furnace. We have also examined the effects of long term storage of the samples both pre- and post-

coarsening in order to determine if the microstructure of the samples will change significantly with time. Finally, in preparation for flight the image analysis system has been upgraded. We are now using a high resolution camera capable of capturing images with a resolution of 3000 x 2000 pixels. This capability reduces errors associated with locating particle interfaces, and increases greatly the number of particles in each image with no loss in resolution.

Microstructural tomography has been used to reconstruct the three-dimensional microstructure of a Pb-Sn solid-liquid mixture from a series of two-dimensional sections. We find that the solid particles form a skeleton which extends throughout the region sampled. These three-dimensional images illustrate the connectivity of the skeleton, including the circuitous and multiple paths through which the particles in the skeleton connect. We find that two particles can contact one another indirectly, via other intervening particles. Chains of particles exist in which all the particles are connected by a grain boundary. These chains can cross-link and intersect, influencing the mechanical stability of the solid skeleton. In addition, these images illustrate the limitations of isolated two-dimensional sections in determining the connectivity of the microstructure, since particles frequently connect out of the plane of a given section. We find that different types of particle contacts are present in the skeleton: grain boundaries, and thin, approximately 1 μm thick, films of liquid. All particles are connected to the skeletal network by such contacts; there are no isolated particles or clusters within the volume probed. In addition, particle shape accommodation is prevalent; the particle morphology is a strong function of the spatial arrangement of the neighboring particles.

The misorientation distribution of the grain boundaries which appear in the Pb-Sn solid-liquid system has been measured. The temporal evolution of this misorientation distribution during coarsening is also being determined. In addition, we measuring the texture of the samples in order to determine if there is a preferred crystallographic orientation of the particles within the sample. These measurements are being done in concert with quantitative metallographic measurements of the volume fraction of solid as a function of time, particle shape and degree of particle sedimentation. This work is in progress and will be completed prior to flight in order to provide a basis of comparison to the results of the spaceflight experiment.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 1/95 EXPIRATION: 10/97

PROJECT IDENTIFICATION: 963-25-05-10

NASA CONTRACT NO.: NAG3-141

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Seyan, I., Ratke, I., Bender, W., and Voorhees, P.W., Ostwald ripening of solid-liquid Pb-Sn dispersions. Metall. Trans. A, (1996).

Proceedings

Voorhees, P.W., "Coarsening in solid-liquid mixtures." Proceedings of the Microgravity Materials Science Conference, 1996.

Vapor Growth of Alloy-Type Semiconductor Crystals

PRINCIPAL INVESTIGATOR: Dr. Heribert Wiedemeier

Rensselaer Polytechnic Institute

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objectives of this research are: (1) the establishment of experimental trends for the relation between convective flow, mass flux, and crystal morphology; and, (2) the identification of microgravity effects and crystal properties for the ternary semiconductor mercury cadmium telluride (HgCdTe).

For this purpose, thin epitaxial layers of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ will be grown on (100) CdTe substrates during the USML-2 mission to observe the effects of microgravity on the morphology of the substrate-layer interface and of the epitaxial layer.

Task Description:

This experiment requires the hot zone to be 625 °C and the cold zone to be 455 °C. The total duration of the experiment is 16 hours. The ampoule assembly is designed to be 160 mm in length, 18 mm outer diameter, and about 31 grams total weight. A cadmium telluride single crystal and a sapphire disc are used for the epitaxial crystal growth as substrate and substrate support, respectively. Four time intervals are required for crystal growth, namely, heat-up, annealing, growth, and cool-down periods.

Identical experiments, except for the level of gravity, are performed on the ground and in space to provide a direct comparison of results.

Task Significance:

The lateral and axial compositional homogeneity (distribution) of the major and dopant components is expected to be more uniform for the space-grown epitaxial layers. The density of dislocations, of strain-induced defects, and possibly the number of inclusions are expected to be considerably reduced relative to ground-control specimens.

In addition, observations of the effects of reduced gravity on the formation of defects at the growth interface and on the propagation of these "birth defects" into the layer are of basic scientific and technological significance.

Progress During FY 1996:

The primary purpose of the USML-2 experiments was to observe the effects of microgravity on the morphology of the substrate/layer interface and of the layer surface for thin epitaxial $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ layers grown on (100) CdTe substrates.

Two epitaxial growth experiments were performed during the USML-2 mission employing growth periods of 1.5 and 2.5 hours.

The results to date of the post-flight analysis and characterization efforts show that the growth islands (shorter growth time) and layer (longer growth time) obtained in microgravity environment are high quality single crystals. The morphology of the as-grown surfaces of the layer and of the islands obtained in space is considerably improved relative to those of ground-based test samples. The compositional microhomogeneity of the epitaxial layer grown during the USML-2 flight is significantly better than those of the deposits obtained on ground. Considerable improvements are being observed for the morphology of the growth interfaces of the space-grown epitaxial layer and islands relative to those of ground-based specimens.

Additional post-flight GCEL tests have been performed in the flight furnace under the actual time-line conditions of the flight experiments.

The comparative analysis and characterization of the flight and ground test samples are being continued.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 3

TASK INITIATION: 10/90 EXPIRATION: 10/96

PROJECT IDENTIFICATION: 963-35-05

NASA CONTRACT No.: NAS8-397

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Chen, K.T., and Wiedemeier, H. The Temperature-Composition Phase Diagram and the Miscibility Gap of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ Solid Solutions by Dynamic Mass-Loss Measurements. J. Electronic Materials, vol. 24, 405-411 (1995).

Ge, Y.R., and Wiedemeier, H. Characteristics of Island Growth of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ on (100) CdTe Substrates by Chemical Vapor Transport. J. Electronic Materials, vol. 25, 1067-1071 (1996).

Wiedemeier, H., and Ge, Y.R. Transient Behavior of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ Films Deposited on (100) CdTe Substrates by Chemical Vapor Transport. J. Electronic Materials, vol. 25, 1072-1081 (1996).

Wiedemeier, H., and Hutchins, M.A. The Temperature-Composition Phase Diagram of the HgTe-HgI_2 Pseudobinary System on the HgTe Rich Side. Z. anorg. allg. Chem., vol. 622, 157-163 (1996).

Presentations

Wiedemeier, H., and Ge, Y.R. "Transient Behavior of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ Films Deposited on (100) CdTe Substrates by Chemical Vapor Transport." Tenth American Conference on Crystal Growth, Vail, Colorado, August 1996.

Wiedemeier, H., Ge, Y.R., and Hutchins, M.A. "Vapor Growth of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ Epitaxial Films under Normal and Microgravity Conditions." SPIE Annual Meeting, Symposium Space Processing of Materials, Denver, Colorado, August 1996.

The Use of Bioactive Glass Particles as Microcarriers in Microgravity Environment

PRINCIPAL INVESTIGATOR: Prof. Portonovo S. Ayyaswamy

University of Pennsylvania

CO-INVESTIGATORS:

Ducheyne, P.

University of Pennsylvania

Task Objective:

Our overall objective is to formulate "optimum" culture conditions which expeditiously produce a three-dimensional bone tissue-like matrix culture using bioactive glass particles as microcarriers in the simulated microgravity environment of NASA-designed Rotating Wall Vessels. To achieve this goal, it is essential to understand the motion of the microcarriers in the fluid field and the stresses on the microcarriers and cells resulting from the rotation of the vessel and the gravity field. Furthermore, understanding of the diffusive mass transport of different chemical species, specifically nutrition, O_2 , CO_2 , in the cell culture fluid medium is important for the interpretation of cellular responses. Baseline data regarding the response of cells to the carrier material under normal gravity conditions are essential in order to uniquely identify the beneficial effect of the carrier material in microgravity culture conditions. It is also necessary to adapt the bioactive glass particles, specifically their morphology, pore size, and porosity to make them suitable as microcarriers on which cells express the osteoblastic phenotype and to promote bone-like formation in a rotating culture vessel. These goals will be achieved over the 1995-1999 four-year research program. This undertaking involves both numerical and experimental aspects.

Task Description:

Experimental Study

The appropriate density and porosity of the bioactive glass (in both the melt-derived and sol-gel-derived condition) will be modified such that the particles remain suspended within the culture-fluid medium in the rotating-wall vessel (RWV) during the entire duration of cell culture. It is only by ensuring that the microcarrier remains suspended in the ambient fluid that we can be certain of microgravity conditions. Microcarrier/cell attachment to the wall of the vessel will negate conditions required for microgravity. Other forms of glass templates for bone tissue formation will also be attempted, specifically, a mat form using glass fibers and sol-gel glass coated polymer beads. Various material characteristics of glass particles will be examined, including chemical composition, morphology, porosity, density, surface modification, and protein absorption. The primary cell type to be studied will be neonatal rat calvaria osteoblasts.

Analytical/Numerical Study

The dynamics of the microcarrier in the RWV will be investigated taking into account a) the effect of spin-up process, b) the influence of the vessel outer wall, and c) multiple microcarrier interactions. The average pressure and the average shear stress on the microcarriers/cells will be evaluated. The transport of chemical species in the fluid by diffusion and convection will be modeled.

Task Significance:

In reconstructive surgery, repair of large bone defects is a major reparative problem. Approaches to bone repair include utilization of autografts or allografts. With autografts, limitations include donor site morbidity, limited donor bone supply, anatomical and structural problems, and elevated levels of resorption during healing. Allografts have the disadvantage of eliciting an immunological response due to genetic differences, and with their use, there is the risk of inducing transmissible diseases. Considerable attention has also been directed at the use of synthetic grafts, most notably hydroxyapatite (HA) and tricalcium phosphate ceramics. However, since it is often desirable to have graft material that will eventually resorb, leaving space for new bone formation, the very low resorbability of stoichiometric HA is considered to be a limiting factor. Using *in vitro* synthesized bone tissue with marrow cells obtained from the patient is an appealing idea to avoid the profound limitations of biological and synthetic grafts. Bioactive glass, a synthetic material with documented extensive bone bioactivity properties, represents a material that optimally combines the requirements of the ideal template for *in vitro* synthesis of bone tissue. Our

investigations with osteoblast growth on bioactive glass bead microcarriers in rotating wall vessels will enable us to establish optimal operating criteria for expeditiously producing three-dimensional bone cell tissue growth under microgravity conditions. Such tissue growth will have wide clinical applications. The development of an improved, more rugged bone tissue that may be used for implantation to correct skeletal disorders and bony defects (such as osteoporosis, fracture healing, and craniofacial abnormalities) will make major contributions to the medical field. Moreover, it may provide therapy for diseases of the bone which occur at unit gravity, provide aid to grown bones in required shapes, and replace or supplant bone that is missing due to birth defects or trauma. In addition, an understanding of the fundamental changes that occur to bone tissue under simulated microgravity could yield important information that will help in preventing or minimizing astronaut bone loss, a major health issue with travel or stay in space over long periods of time.

Progress During FY 1996:

Experimental Study:

During the year 1995-1996, we have investigated the effect of bioactive glass on bone cell function under normal gravity conditions in order to establish base-line data as a reference for our future studies under microgravity conditions. Porous bioactive glass disks with a porosity of 28% and a pore size of 70-200 nm were treated using a previously developed two-step process to optimize surface conditions for bone formation. In the first step, the glass is immersed in tris buffer supplemented with ions in concentrations similar to the interstitial fluid to form a calcium phosphate-rich layer at the glass surface. Then the glass is immersed in tissue culture medium supplemented with 10% serum to absorb serum proteins that provide sites for cell attachment. ELISA and Western blot techniques revealed that the presence of Ca-P layer on bioactive glass promoted the adsorption of fibronectin, which might contribute to the enhanced cell adhesion on the bioactive glass. Neonatal rat calvaria osteoblasts were seeded on the surface-modified bioactive glass, and various markers for the osteoblastic phenotype were assayed at time points ranging from 3 to 14 days. Cells seeded on bioactive glass exhibited phenotypic characteristics typical for the osteoblastic function. High numbers of cells colonized the bioactive glass surface and produced collagen type I and III, osteopontin and bone sialoprotein, expressed high alkaline phosphatase activity, and formed a significant quantity of bone-like tissue. Both morphological and biochemical analysis demonstrated that the osteoblasts formed a calcified tissue exhibiting many of the major characteristics of bone.

We have also fabricated melt-derived and sol-gel derived glass particles (S70) to be used as microcarriers. We have transformed the silica-based, Ca, P-containing glass granules into CaP-shells by differential immersion of the glass granules in physiological solution(s). The immersion conditions (i.e., solution composition, timing and a number of solution exchanges, material weight to solution volume ratio, W/V, etc.) were varied in order to allow the following reactions to occur: 1) formation of a surface CaP layer; 2) continuous silica-network dissolution, remaining under the CaP layer, until 80 to 100% of the original Si content in the glass is dissolved. In order to stimulate the continuous silica network dissolution, the solution(s) used for the immersion experiments were undersaturated with respect to soluble silica.

We have also studied the motion of a 1 mm diameter particle with density 1.05 g/cm³ in a Rotating Wall Vessel (HARV, 10ml, Synthecon, Inc.) filled with water. The experimentation was carried out at various rotational speeds and initial particle positions. We have found that the trajectory of the particle was an outward spiral, similar to the one predicted by the numerical model. Furthermore, the data has also shown that the time for the particle to reach the wall is a function of the angular velocity. For a three-dimensional bone cell culture to develop, it is preferable that the microcarrier materials remain dispersed within the boundary of the culture vessel walls during the cell culture period and generally maintain their position in the fluid flow field. Our numerical and experimental studies with a single particle have shown that density difference between the microcarrier and the fluid is a key factor for maintaining the particle in the medium within the boundary of the culture vessel. Since the usual bioactive glass has a density greater than that of a standard culture medium, an adaptation of the glass carrier material is necessary for it to be usable in a microgravity environment.

Numerical Study:

We have developed a numerical solution to the problem of fluid flow and particle motion in a rotating bioreactor containing a single rigid spherical microcarrier particle. It is assumed that the flow field is not affected by the presence of the particle. At every instance, the fluid is assumed to be in solid body rotation at the instantaneous angular velocity of the vessel. Secondary flows are ignored and the flow is considered to be steady ("spin-up" is

considered to be negligible). The acceleration of the fluid due to the presence of the particle is accounted for by the virtual mass concept. Based on the above assumptions, we have derived the equations for the trajectory of the microcarrier in both inertial and rotational frames.

The numerical analysis shows that when the particle density (ρ_p) is less than that of the fluid (ρ_l), the particle ends up at an equilibrium position in the inertial reference frame, while in the rotating frame it moves, subsequent to the decay of the transient motion, on a circular trajectory concentric with the axis of rotation. On the other hand, when the particle density is larger than that of the fluid ($\rho_p > \rho_l$), the particle migrates towards the outer wall while it is rotating in the fluid and eventually intercepts the outer wall. When $\rho_p > \rho_l$, the time for the particle to intercept the outer wall (t_w) has been calculated as a function of vessel angular velocity (W), the viscosity of the fluid (μ), the density difference between the particle and the fluid ($\Delta\rho$), particle radius (a), and initial position of the particle (R_0, q_0). This is of interest because most microcarrier particles are likely to be denser than the fluid. The results of the numerical analyses are summarized below. In each case described, all parameters except the one under consideration have been held constant.

Effect of angular velocity (W): At relatively high rotating speeds, t_w decreases with the increase of angular velocity, W .

Effect of viscosity of the fluid (μ): The time t_w increases with μ in an essentially linear manner.

Effect of density difference ($\Delta\rho = \rho_p - \rho_l$): The time t_w decreases with the increase of $\Delta\rho$.

Effect of particle size (a): The time t_w decreases with the increase of the particle radius, a .

Effect of the initial position of the particle (R_0, q_0): The time t_w decreases with the increase of the initial distance from the rotation axis. This is as would be expected.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 7/95 EXPIRATION: 7/99

PROJECT IDENTIFICATION: 962-23-01-23

NASA CONTRACT NO.: NAG9-817

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Ducheyne, P., Schepers, E., and Shapiro, I. Bone bioactive material surface changes and bone cell function are related. *Bioceramics 9*, Ed. T. Kokubo, Elsevier, Oxford, England, (1996).

El-Ghannam, A., Ducheyne, P., and Shapiro, I. Porous bioactive glass and hydroxyapatite stimulate bone cell function in vitro along different time lines. *J. Biomed. Mater. Research*, (In Press).

Presentations

Ducheyne, P. "The Use of Bioactive Glass Particles as Microcarriers in Microgravity Environment." Biotechnology Program, Investigators Working Group meeting, Houston, Texas, February 1996.

Ducheyne, P., Gao, H., El-Ghannam, A., Shapiro, I., and Ayyaswamy, P. "The use of bioactive glass particles as microcarriers." International Mechanical Engineering and Exposition, Atlanta, GA 1996.

Evaluation of Ovarian Tumor Cell Growth and Gene Expression

PRINCIPAL INVESTIGATOR: Jeanne L. Becker, Ph.D.

University of South Florida

CO-INVESTIGATORS:

Spaulding, G.F.

NASA Johnson Space Center (JSC)

Widen, R.H.

University of South Florida (Tampa Gen. Hospital)

Task Objective:

The overall objective of this project is to examine the growth and gene expression of LN1 ovarian tumor cells grown three-dimensionally in the NASA Rotating-Wall Vessel (RWV).

The Specific Aims proposed to accomplish this objective were as follows:

1. To characterize the growth and gene expression of ovarian tumor cells cultured in the RWV, relative to conventional *in vitro* kinetics.
2. To evaluate ovarian tumor cell oncogene expression in cells grown in the RWV.
3. To determine if specific changes in oncogene expression in tumor cells cultured in the RWV can be correlated with alterations in other parameters of cell growth.
4. To examine whether tumor cell growth in the RWV produces alterations in the cell cycle.
5. To investigate hormonal modulation of ovarian tumor cells grown in the RWV.

Task Description:

The purpose of this research is to develop an *in vitro* model for the growth of ovarian tumor cells. The unique features of this model are (a) maintenance of tumor cell characteristics expressed *in vivo*, (b) complex three-dimensional tissue-like growth, and (c) the opportunity to sample tumors at multiple time points during three-dimensional development without serial massaging which may result in the loss of previously expressed cellular characteristics. The knowledge gained from this model of ovarian tumor will be used to examine growth characteristics and hormonal responsiveness of other human gynecologic tumors.

Task Significance:

The study of human cancer has been limited by the unavailability of reliable *in vitro* models to support long-term growth and cellular differentiation. Studies have shown that maintenance of three-dimensional architecture can significantly influence tumor cell gene expression, chemotherapeutic resistance, and tumor antigen expression, relative to cells grown two-dimensionally as a monolayer.

We have developed a model of human ovarian cancer using the LN1 ovarian tumor cell line. LN1 was derived from a heterologous mixed müllerian tumor of the ovary which was composed predominantly of a poorly differentiated mesenchymal component with a smaller carcinoma element. Grown as a monolayer, LN1 cells exhibit a carcinomatous phenotype. However, grown as three-dimensional tissue-like aggregates in the NASA RWV, LN1 exhibits multiple cell populations of both epithelial and mesenchymal phenotype as exist in these tumors *in vivo*. Moreover, proto-oncogene expression patterns differed within individual cell populations generated during three-dimensional growth. When the cell populations generated in three-dimensional culture are placed back into monolayer, they revert to the carcinomatous phenotype. These findings support the Combination Theory which suggests that the multiple malignant cells comprising mixed müllerian tumors arise from a single stem cell. We hypothesize that LN1 represents such a stem cell, and that the RWV three-dimensional culture system provides the conditions necessary for the differentiation of LN1 into multiple cell types as were present *in vivo*.

Progress During FY 1996:

Over the past four years, we have used the NASA Rotating-Wall Vessel (RWV) to develop an *in vitro* model for the study of human ovarian tumor. Using this three-dimensional culture model, we have gained a significant understanding of the growth and differentiative capacity of LN1 ovarian tumor cells. The results of this work were published in three manuscripts and an extended abstract. During our previous years of funding for this project, we have satisfied the stated specific aims as follows:

- (a) **Characterization of the growth of LN1 cells in the RWV relative to conventional monolayer culture.** This included determination of the metabolic activity during three-dimensional growth and definition of media requirements for optimal three-dimensional development. In addition, we described the ability of LN1 to undergo significant differentiative events leading to the generation of multiple subpopulations of cells exhibiting distinct phenotypic characteristics.
- (b) **Evaluation of LN1 oncogene expression during three-dimensional growth.** We described the expression of cellular oncogenes HER2/neu, H-ras, K-ras and p53, and corresponding proteins p185^{HER2^{neu}}, p21^{H-ras}, p21^{K-ras}, and mutant p53 protein. In addition, we examined TGF- β 1 expression and found it to be significantly modulated as a function of three-dimensional development.
- (c) **Determination of whether specific changes in oncogene expression during three-dimensional growth, relative to monolayer culture, correlated with changes in other parameters of LN1 growth.** We described that differentiation of LN1 into multiple distinguishable cellular subpopulations during extended three-dimensional growth as multicellular aggregates correlated with differences in the expression of oncoproteins p21^{H-ras}, p21^{K-ras}, and mutant p53 protein within these individual subpopulations.
- (d) **Examination of cell cycle laterations during three-dimensional growth.** We described that LN1 undergoes an increase in resting (G_0/G_1) cells with a concomitant decrease in proliferating cells (S and G_2 +M phases) during extended three-dimensional development.
- (e) **Investigation of hormonal modulation of LN1 growth.** We found that estrogen and progesterone are mildly growth inhibitory for LN1. The study of hormonal modulation of LN1 growth required that we develop a new culture media which lacked hormone activity. We have developed such a media which is a modified form of the GTSF media used to grow LN1 in the RWV. This media lacks phenol red, which has been shown to exhibit estrogenic activity in some culture systems and which also utilizes charcoal adsorbed fetal bovine serum (to remove trace amounts of hormones which can be present in the serum). We find similar growth characteristics of LN1 in both GTSF and our modified form of GTSF.

During our fourth year of funding, we have further investigated hormonal modulation of LN1 growth. Because LN1 cells are a multiple drug-resistant ovarian tumor cell line, we also initiated pilot studies to examine chemotherapeutic effects on LN1 growth. Treatment of these cells with the antiprogesterone agents mifepristone (RU486) or onapristone (ZK98299) was found to induce growth inhibition greater than that achieved with progesterone. We found similar growth inhibitory effects of the antiprogesterone agents on Ishikawa human endometrial carcinoma cells. Moreover, combination treatment of the endometrial cancer cells with antiprogesterone and progesterone induced significantly greater inhibition of cell growth.

Because RU486 has been shown to be capable of modulating drug resistance via regulation of multidrug resistance gene (mdr1) expression, we also examined mdr1 expression in LN1 and found the cells to express mRNA as well as the mdr1 gene product P-glycoprotein during three-dimensional growth. Furthermore, preliminary studies also suggest that treatment with antiprogesterone is able to reverse the taxol resistance of LN1 cells. We hypothesize that this effect may occur via alteration of mdr1 expression in these ovarian tumor cells since one mechanism of taxol resistance is mediated via mdr1 P-glycoprotein. As such, we have submitted a renewal grant application on this project to further investigate mechanisms whereby antiprogesterone may modulate drug resistance in LN1 ovarian tumor cells. Because chemotherapeutic resistance *in vitro* is influenced directly by the spatial orientation of the growing cells, culture of LN1 as three-dimensional multicellular aggregates in the NASA RWV represents a particularly relevant model to examine mechanisms of drug resistance in these human ovarian tumor cells.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 11/92 EXPIRATION: 11/95

PROJECT IDENTIFICATION: 962-23-01-15

NASA CONTRACT No.: NAG-648

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Arango, H., Satyaswaroop, P., Cavanagh, D., Goldrain, V., and Becker, J. Effects of 17 beta-estradiol and mifepristone (RU486) on Ishikawa human endometrial cancer cell line. *Am. Assoc. Cancer Res.*, No. 2231, (1996).

Arango, H., Satyaswaroop, P., Cavanaugh, D., and Becker, J. The growth inhibitory effects of onapristone (ZK98299) and mifepristone (RU486) on Ishikawa human endometrial cancer cell line. *West. Assoc. Gynecol. Oncol.*, (1996).

Becker, J.L., Papenhausen, P.R., and Widen, R.H. Cytogenetic, morphologic and oncogene analysis of a cell line derived from a heterologous mixed müllerian tumor of the ovary. *In Vitro Cell. Develop. Biol.*, (In Press).

Goodwin, T.J., Prewett, T.L., Spaulding, G.F., and Becker, J.L. Three-dimensional culture of a mixed müllerian tumor of the ovary: expression in vivo characteristics. *In Vitro Cell Develop. Biol.*, (In Press).

Pinelli, D., Cavanagh, D., and Becker, J. Hormonal modulation of Ishikawa cells during three-dimensional growth in vitro. *Soc. Gynecol. Oncol.*, (Submitted).

Presentations

Becker, J. "The benefits of space research on women's health." Annual meeting of the Society for Women Engineers, Melbourne FL, 1996.

Becker, J. "Hormonal modulation of human endometrial carcinoma growth." NASA-JSC Investigatory Working Group, Meeting, 1996.

Expansion and Differentiation of Cells in Three-Dimensional Matrices Mimicking Physiological Environments

PRINCIPAL INVESTIGATOR: Prof. Rajendra S. Bhatnagar

University of California, San Francisco

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Our overall objective is to develop 3-D culture systems for mammalian cell cultures based on materials that mimic type 1 collagen, a major component of the extracellular matrix (ECM). We have identified a potent cell binding domain of type 1 collagen. Synthetic compounds based on this domain, as well as several conformational analogue peptides, exhibit many of the cell directed activities of collagen including the ability to attach cells and to promote their migration into several 3-D matrices. In this environment, cells exhibit remarkable differentiated behavior.

Task Description:

We expect to perform the following tasks in FY 1996:

1. Prepare and characterize synthetic matrices containing a synthetic fifteen-residue peptide analogue (P-15) of a cell-binding domain of collagen. In this project period, we propose to synthesize, characterize, and examine composites of P-15 with porous hydroxyapatite, polyglycolate ester fibers, and hydroxypropyl methylcellulose (HOPMC) hydrogels.
2. Determine the biological activity of the matrices in terms of cell-binding and differentiation. We will examine the binding and differentiation of dermal fibroblasts and HOS (human osteosarcoma) cells and initiate studies on the binding and differentiation of liver and breast derived cells.

Task Significance:

The proposed research will help in designing more efficient bioreactors by attaching cells in 3-D matrices via receptors for ECM. Since a cell in its native physiological environment is surrounded by the ECM and by other cells and receives informational messages from both the ECM and from the surrounding cells through specific receptors, and since collagen is presumed to be the primary transducing agent for mechanical signals transmitted through specific receptors, the synthetic environment proposed by us will promote the expansion of cell populations in a differentiated state. Such matrices can be engineered to allow for a facile exchange of nutrients and wastes with a surrounding medium. Cultures in such matrices will (i) facilitate expansion of differentiated cell populations, (ii) allow closer examination of the role of geometry and surroundings (ECM, cells) on differentiation, (iii) allow the determination of the role of mechanical signals in differentiation through the manipulation of applied force, and thus (iv) make possible the optimization of culture conditions for bioreactors.

Progress During FY 1996:

During the Period of the Report, the following matrices were made as composites with peptides: (i) Hydroxyapatite-Peptide, (ii) polyglycolate-peptide, (iii) hydroxypropyl methylcellulose-Peptide.

The following cell cultures were established: (i) Neonatal human dermal fibroblasts, (ii) Bond cell lines MG-63, SaOS-2, U2OS and HOS, (iii) Liver cell lines Chang liver cells, SK-HEP1 human adenocarcinoma, HEP-G2 human liver tumor, (iv) Human breast cell lines Ductal carcinoma, MDA-MB-231 adenocarcinoma, HBL-100, normal cells.

3-D growth and differentiation of (i) dermal fibroblasts in Hydroxyapatite-Peptide, polyglycolate-peptide, and hydroxypropyl methyl cellulose-Peptide and (ii) HOS cells on Hydroxyapatite-Peptide are currently under investigation. Our studies show the formation of 3-D colonies and differentiation of dermal fibroblasts into an osteoblast-like phenotype on Hydroxyapatite-Peptide matrix. HOS cells also showed increased attachment and differentiation on composites of Hydroxyapatite-Peptide. Differentiation was examined by monitoring the expression of bone-related genes (type 1 collagen, collagenase, TGF-b, osteonectin) in these cells. In addition, we

observed transient expression and secretion of alkaline phosphatase, and transient expression of BMP-7. These observations support our concept that suspending cells in composites with a 3-D distribution of ligands for collagen receptors is likely to facilitate 3-D colony formation and differentiation.

Dermal fibroblasts retain fibroblast characteristics on polyglycolate-peptide. Gene expression studies are on going in these cultures. Our preliminary observations suggest that attachment of fibroblasts to P-15-containing matrices facilitates the transmission of mechanical forces such as those generated by fibroblast contraction. These cultures are being adapted for the study of mechanical signaling of cells and subsequent differentiative events.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/95 **EXPIRATION:** 8/99

PROJECT IDENTIFICATION: 962-23-01-35

NASA CONTRACT No.: NAG9-812

RESPONSIBLE CENTER: JSC

Quantitative, Statistical Methods for Pre-Flight Optimization, and Post-Flight Evaluation of Macromolecular Crystal Growth

PRINCIPAL INVESTIGATOR: Dr. Charles W. Carter

University of North Carolina, Chapel Hill

CO-INVESTIGATORS:

Ducruix, A.
Ries-Kautt, M.CNRS-Gif Laboratoire de Biologie Structure
CNRS-Gif Laboratoire de Biologie Structure

Task Objective:

To generalize the application of response surface methodology to a broad range of crystallization studies. To develop and provide tutorial workshops to distribute skills in designing response surface experiments and analyzing the resulting data for stationary points. To rationalize the space of experimental parameters used in the study of crystal growth and to map the behavior of model systems onto this parameter space using response surface analysis.

Task Description:

This approach involves making and testing models of crystal growth which involve quadratic polynomials, which are the simplest mathematical functions that can pass through a maximum or minimum. Because these are slowly varying mathematical functions, they are most appropriate for modeling a local neighborhood of a maximum or minimum value for the response a system makes to changes in the independent parameters. The polynomial form of the functions facilitates estimation of a small number of coefficients using a minimum number of experiments.

It is also a simple matter to determine the coordinates of the optimum point by partial differentiation and solution of the resulting simultaneous equations. The model and its statistical descriptors become a valuable set of scientific documentation. The coefficients of response surface descriptions of crystal growth, together with their statistical significance, afford an excellent source of experimental evidence regarding its dependence on experimental parameters. Moreover, working at stationary points also enhances the reproducibility of experiments, because of the property that the partial derivatives vanish at stationary points of the quadratic function.

Task Significance:

A generally applicable protocol for determining that the conditions for crystal growth correspond to an optimum in the response surface will extend the value of flight-based microgravity experiments, by helping to assure that experiments are minimally vulnerable to experimental errors and hence as reproducible as possible. By eliminating experimental fluctuations as an important source of variation, this in turn will enhance the signal-to-noise ratio of all microgravity experiments done under optimal conditions. Ultimately, the same experimental strategy can be extended to the study of crystal diffraction quality. This work may therefore contribute to improvements in the detail with which protein structures can be analyzed, as well as the quantitative attribution of such improvements to microgravity.

Analysis of model systems in this way can provide an experimental map of crystal growth in a rational, multidimensional parameter space and, potentially, valuable evidence regarding the existence and utility of "generic" phase diagrams for crystal growth.

Progress During FY 1996:

We have arranged for Robert Cudney of Hampton Research, Inc., to provide five proteins of his choosing, for which we will determine analytical response surfaces, to generalize the approach to as broad a selection of proteins as possible. I have hired a research specialist experienced in protein crystal growth, who will join the lab December 1, 1995 to supervise the project. Once she has learned to carry out response surface experiments, we will schedule and advertise the first of several workshops to teach the techniques to protein crystallographers involved in NASA microgravity research. As part of the theoretical development of the method, I formally derived a local approximation to supersaturation, applicable to any situation where estimates exist for the limiting solubility in the absence of crystallizing agent and the exponential decay constant for the dependence of solubility on the crystallizing agent concentration. This approximation facilitates a direct coordinate transformation for the solubility phase

diagram, making it possible to represent the nucleation zone as a rectangle and to place experiments on a rectangular grid. Though apparently abstract, this result has important practical advantages. It will help to assure that sampling for response surface experiments can be done in as efficient a manner as possible with minimal loss of data through inadvertent placement of experiments that do not crystallize and hence do not contribute to the analysis.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 0

TASK INITIATION: 7/95 EXPIRATION: 6/99

PROJECT IDENTIFICATION: 962-23-08-31

NASA CONTRACT NO.: NAG8-114

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Carter, Jr., C.W. A Local Approximation to Supersaturation Affords a Useful Coordinate Transformation for the Study of Crystal Growth. *Acta Crystallographica*, vol. D52, 647-654 (1996).

Yin, Y., and Carter, Jr., C.W. Incomplete Factorial and Response Surface Methods in Experimental Design: Yield Optimization of tRNA^{Trp} from in vitro T7 RNA Polymerase Transcription. *Nucl. Acids. Res.*, vol. 24, 1279-1287 (1996).

Microgravity Simulated Prostate Cell Culture

PRINCIPAL INVESTIGATOR: Prof. Leland W. Chung

University of Virginia

CO-INVESTIGATORS:

Zhau, H.E.
Chang, S.M.
Gotoh, A.University of Virginia
University of Virginia
University of Virginia

Task Objective:

Prostate cancer is the most common malignancy found in the United States. In 1994, it was estimated that 200,000 new cases of prostate cancer will be diagnosed. This accounts for over 32% of all cancer cases detected and is the second leading cause of death in American men. As an endocrine organ, the prostate gland is highly responsive to the steroid androgen, which induces growth and differentiation *in vivo*. Consequently, endocrine therapy remains the leading therapeutic modality for the treatment of local and metastatic disease. Unfortunately, an escape of the blockade by androgen antagonists presents a serious threat to the success of endocrine therapy. Despite much effort in the past years to develop model systems to study the effects of androgen on prostatic epithelial cell growth and differentiation *in vitro*, there is little evidence that prostate epithelial cells respond directly to the mitogenic signal of androgen. One of the key reasons that these attempts have failed is the conventional prostate cell culture system will not retain an essential feature of the prostate gland, i.e., a 3-dimensional organization composed of interactive prostate stromal and epithelial cells. The purposes of this investigation are to establish a valid cell culture system for the study of *in vivo* growth control mechanisms in the prostate gland and to identify and characterize the key players, growth factors, their receptors, and extracellular matrices in microgravity-simulated conditions.

Task Description:

The central theme of this proposal is to establish a 3-dimensional cell-cell interaction model *in vitro* to examine the influence of androgen, known and novel growth factors, extracellular matrices, and differentiating agents on the growth and differentiation of human prostate cancer. To accomplish this goal, we propose to pursue the following three objectives:

First, we propose to construct 3-dimensional prostate organoids *in vitro* under microgravity-based conditions. We will compare the growth and differentiative potentials of the prostate organoids formed through cell-cell interactions between prostate stromal cells obtained from normal, benign, or cancerous prostate and epithelial cells derived from normal prostate or the LNCaP cell line (which is derived from a human prostate cancer lymph node deposit). These comparisons will help us to understand the possible regulatory roles of prostate stromal cells on prostate epithelial growth and differentiation.

Second, we will test the biologic behaviors and the functionalities of the reconstituted prostate organoids. The growth and differentiative responses of the reconstituted prostate organoids to androgen (dihydrotestosterone, DHT), growth factors (transforming growth factor α , TGF α ; transforming growth factor β keratinocyte growth factor, KGF; hepatocyte growth factor/scatter factor, HGF/SF; and basic fibroblast growth factor, bFGF), extracellular matrices (plasma membrane preparation from human prostate stromal cells, collagen IV, laminin, fibronectin, heparan sulfate proteoglycans, and Matrigel R), and differentiating agents (phenylbutyrate, retinoid fenretinide) will be evaluated by histomorphologic, immunohistochemical, biochemical, and molecular methods. This microgravity-simulated model system may be developed and perfected for future use as a standard for drug screening programs and could serve as a valuable tool to complement existing animal model systems.

Finally, because of the possible parallelism of prostate growth and differentiation between the microgravity-simulated conditions and *in vivo* conditions, we propose to use this system to produce large quantities of potentially biologically relevant molecules that can be used to stimulate human prostate epithelial cell growth *in vitro* using conventional culture conditions on plastic dishes. It is hoped that the enriched source of these biologically relevant factors will assist our future attempts to purify, characterize, and close factors that may be useful in evaluating the possible roles of these factors in the clinic progression of human prostate cancer.

Task Significance:

The specific significance of this proposal involves the delineation of central questions in prostate cancer research.

(1) Although the prostate gland is a highly androgen-responsive organ, why do prostate cells, when cultured *in vitro*, generally not show growth responses to androgens? Despite the coculture of prostate epithelial cells with prostate fibroblasts, androgen only induces marginal growth responses in the cultured prostate cells *in vitro* (Chang and Chung, 1989).

(2) What are the physiological mediators for androgen-induced prostate growth responses?

(3) Can the growth mediators alone or differentiating agents promote prostate cancer differentiation under chemically defined cell culture conditions? With respect to question 1, there has been considerable speculation on the interrelationship of structure and function of the prostate gland. Reciprocal interaction between prostate stroma and epithelium, under proper configurations (e.g., 3-dimensional structure), may determine the differentiated function of prostatic sinus epithelium. Tissue recombinants composed of fetal UGM and UGE (urogenital sinus epithelium) have been demonstrated to undergo normal prostatic morphogenesis and cytodifferentiation when promoted by androgen (Cunha and Chung, 1981; Chung and Cunha, 1983) and selected growth factors (Chung, et al., 1992; Sugimura et al., 1994) both *in vivo* and *in vitro*. These results illustrate the importance of proper organization and orientation of prostate stroma and epithelium; a 3-dimensional organization could be prerequisite for the androgen-induced growth and differentiation observed in the normal prostate gland.

Progress During FY 1996:**Introduction and Objectives:**

A three-dimensional model for the study of stromal-epithelial interaction was established in our laboratory. This model involves the co-culture of LNCaP cells with either human prostate or bone fibroblasts in microgravity-simulated culture conditions. It is known that stromal-epithelial interaction plays a key role in normal prostate development and its neoplastic progression. In previous publications, we demonstrated that stromal-epithelial interaction under microgravity-simulated conditions resembles the behaviors of the prostate gland grown *in situ*. Since organ-specific fibroblasts (bone and prostate) have been demonstrated to induce marginally tumorigenic LNCaP cells to form solid PSA-secreting tumors *in vivo* through cell-cell interactions, and organ-specific fibroblasts have been shown to be capable of promoting the acquisition of androgen independence and metastatic potential in prostate cancer cells, we have begun to construct a three-dimensional model system to study the interaction between human prostate or bone fibroblasts under microgravity-simulated culture conditions. Results of these studies shown that, unlike the *in vitro* co-culturing of interactive cell types of plastic dishes, microgravity-simulated cell culture conditions promote LNCaP cells to secrete PSA in an androgen-dependent and antiandrogen (Casodex)-antagonized manner when tested in the co-cultured microgravity-simulated conditions.

Methods:

In these studies, LNCaP cells, alone or accompanied by 5X106 human prostate (Pf) or bone MS or SAOS-2) fibroblasts, were loaded into a 55ml microgravity rotating vessel containing 55 mg of Cytodex-3 microcarrier beads. The PSA production, histomorphology, and the rate of cell proliferation were analyzed in the condition medium and in specimens recovered from the rotating vessel.

Results:

We have shown that microgravity-simulated co-culture of LNCaP and prostate or bone fibroblasts mimic *in vivo* conditions and result in facilitating interaction between stromal and epithelial cells. While SAOS-2 cells stimulated rapid PSA production by LNCaP cells, MS suppressed similar PSA production by LNCaP cells. Pf, however, induced both LNCaP cell growth and PSA expression. Pf was further demonstrated to enhance the invasive properties of the LNCaP cells. Similarly co-cultured Pf and Lncap cells on plastic, however, failed to induce the invasive property of LNCaP cells.

Conclusions:

These studies allow us to conclude that microgravity-simulated cell culture conditions preserve the in vivo three-dimensional organization of prostate epithelial and stromal cells, although both prostate and bone fibroblasts failed to produce tumor progression when co-cultured with LNCaP cells on plastic dishes. The prostate fibroblasts can facilitate tumor progression under these microgravity-simulated conditions, possible through the mechanism of forming a three-dimensional interactive organoid involving active reciprocal communication between prostate fibroblasts and epithelial cells. In summary, our data suggests that prostate fibroblasts, when interacting with LNCaP cells under microgravity simulated conditions, facilitate the formation of three-dimensional architecture and confer tumorigenic, as well as induced potential within LNCaP cell phenotypes.

In the past year, our laboratory relocated from the University of Texas M. D. Anderson Cancer Center to the University of Virginia Health Sciences Center on November 1, 1995. The laboratory is currently full functional.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/95 EXPIRATION: 9/99
PROJECT IDENTIFICATION: 962-23-01-19
NASA CONTRACT No.: NAG9-823
RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Zhau, H.E., Goodwin, T.J., Chang, S.M., Baker, T.L., and Chung, L.W.K. Establishment of a 3-dimensional human prostate organoid co-culture under microgravity-simulated condition: Evaluation of androgen-induced growth and PSA expression. In Vitro, In Press, (July 26, 1996).

Noninvasive Near-Infrared Sensor for Continual Cell Glucose Measurement

PRINCIPAL INVESTIGATOR: Dr. Gerard L. Cote

Texas A&M University

CO-INVESTIGATORS:

Rastegar, S.

Texas A&M University

Task Objective:

The specific objectives of this four-year research project are:

1. Maximize the glucose signal while minimizing the water absorption peak with a bench-top NIR system for predicting glucose concentration.
2. Develop digital filter pre-processing computer algorithms coupled with multivariate calibration techniques applied to the NIR spectra to quantify glucose concentrations for the cell culture medium.
3. Design, build, and test the delivery/collection system to maximize the NIR signal in a rotating-wall vessel.

The first two specific aims were the focus of the first year.

Task Description:

For this investigation, a plan was forwarded to accelerate the development of a three-dimensional tissue culture system by building on previous data toward the design of an on-line, non-invasive, near-infrared (NIR) optic sensor for use with the rotating-wall bioreactors. The primary focus is to develop the technology for continuously and non-invasively sensing glucose in the cell culture media to allow for long-term, on-line monitoring without potential contamination of the medium from invasive approaches.

To date, the required advances for NIR spectroscopy to be a quantifiable indicator of cell culture glucose are novel techniques in order to achieve a stronger, more accurate, and repeatable signal which compensates for cell culture medium variations and can be miniaturized for use with the rotating-wall vessels and space applications.

Task Significance:

The culturing of a variety of tissues under clinostatic suspension in rotating vessels has been enhanced by NASA's biotechnology program. Increased cell viability, adhesion, tissue formation, and differentiation have been demonstrated. However, to increase the production of cell cultures, the design of bioreactors must include computer control of cell culture processes. In order to do this, on-line, preferably non-invasive sensors must be implemented to monitor various parameters of the cell culture and feed back that information for regulation of the environment. One vital parameter of interest is the concentration of glucose in the cell culture media. The basis for cell culture media is an isotonic saline solution of nutrients and cofactors. In a typical medium, glucose is the major carbohydrate energy source. Cell proliferation causes rapid consumption of glucose which in turn causes growth limitations of the cells. Thus, the relative concentration change of glucose is a determining factor for the rate of cell culture growth. By permitting closed-loop control of cell culture glucose, the growth rate will be optimized. Current techniques used to monitor the value of this parameter within cell culture media are invasive and cannot be used in a closed-loop system since they are not on-line measurements. In this research, a near-infrared spectroscopy system is proposed to perform the required glucose measurements on-line and non-invasively, without potential contamination of the cell culture media.

Progress During FY 1996:

A new unique Fourier Transform Infrared (FTIR) spectroscopy system was purchased to perform the initial research which included the capability of delivering spectral wavelengths under software control from the near infrared region (NIR) of 2.0 to 2.5 mm to the mid-infrared region (MIR) of 2.5 to 10 mm without having to change the hardware such as the light source, beam splitter, or detector element. This NIR region is preferred since it contains a minimum for the water absorption signal and three glucose overtone peaks, allows for a longer path length of transmission, and is suitable for use with multivariate statistical technique. Due to the weak glucose bands, it is

difficult to resolve peaks from solutions of low to moderate glucose concentrations, thus we have investigated several modifications of the spectrometer setup in terms of hardware changes relating to specific aim number one and post processing software development which relates to specific aim number two. Lastly, preliminary studies involving effect of pH and temperature on the sample are underway.

Hardware:

1) Increase energy delivered to the sample . One major drawback to FTIR-NIR approaches is the amount of energy that can be delivered to the sample from a source within the machine. This limitation is in part due to heating of the electronics within the device. In our system, a hole was drilled in the chassis of the FTIR bench to allow exterior coupling of light into the interferometer. With focusing optics and a 50W tungsten-halogen lamp with back reflector, we were able to increase the amount of light transmitted through the sample at a wavelength of 2.2 mm by a factor of ten over that given by the factory-installed source.

A tradeoff to the increased throughput was that the dynamic range of the detectors was exceeded and the sample heated. Unlike dispersion-based devices, FT interferometers do not separate the energy into narrow wavelength bands, but instead, all of the light is directed through the sample at the same time, which means the detector responds to the total light intensity incident on its face. To eliminate the problem, a combination of a doped germanium flat and a short-pass filter were used to restrict the light to the desired range. Over the 2.0-2.5 μm range, a minimum of 80% transmittance is realized. This is generally better than available interference filters and is less expensive.

2) Optimize experimental parameters.

Experimental parameters in this system include gain, spectral resolution, mirror velocity, sample pathlength, and number of scans (averaged). A factorial experiment was designed and completed to identify the best combination of settings for prediction of glucose concentration in water. A calibration model was built using scans collected at different settings and the squared error of prediction was taken as the instrument response. Therefore, a minimum SEP was the objective. Parameters were chosen within the known limits of the instrument; for example, we chose mirror velocities between 10 and 50 kHz because the detector response is maximal in that range. The experiment involved the collection of approximately 120 spectra with collection times ranging from a few seconds to nearly an hour. The data collection spanned more than 48 hours.

The results of the analysis did not show a clear "best" choice; however, it did show clear poor choices. The experiment confirmed that the use of more averaged scans decreases error (noise) and also ≤ 2 mm pathlength is necessary. The other parameters did not affect the prediction error significantly. Therefore, we chose the combination of variables that would minimize the scanning time. The results indicate that good performance is depicted given a resolution of 2 cm^{-1} , a mirror velocity of 40 kHz, a gain of 4, a pathlength of 1mm, and 256 signal averages.

Software:

The software development was based on producing a wavelength selection algorithm to determine the minimum number and location of optimal wavelengths that can be used to predict glucose concentration. In a final glucose monitoring device, a key limitation to the hardware will be the light source. It is clear that, although a tungsten-halogen bulb produces the appropriate wavelengths, it is very inefficient with much of the energy outside the region of interest and very broad band. With the development of new semiconductor laser sources in this region, it may be possible to produce a fixed spectrum of coherent light focused on the sample. However, it is important to identify the appropriate wavelength and minimum number of lasers for prediction of glucose concentration.

Glucose-doped water and glucose doped cell culture medium has been used to investigate four different wavelength selection algorithms to identify both the minimum number of wavelengths that can be used without loss in the prediction of the glucose concentration and to determine the optimal wave numbers that are most useful for the determination of glucose within the cell culture media used.

The first method uses spectral features of the absorbance scans to determine a set of initial wavelengths of principal importance. The program ranks these features by size and then tests the top n initial and $2m$ adjacent wavelengths to arrive at an optimal set of wavelengths.

A second selection method is based upon the work of Brown and Spiegelman¹. Using a simple linear regression of the form,

$$\gamma_{kj} = \alpha_j + \beta_j \chi_k + \varepsilon_{kj}$$

where j represents the individual wavelengths and k represents observations, the method sorts the absolute values of β_j / σ_j . In this formulation, σ_j is an estimate of the error standard deviation at a particular wavelength. The wavelengths represented by the highest n of these values are selected. The value of n is selected to minimize a confidence interval.

The last two methods are 'step-down' and 'step-up' procedures, respectively. That is, the former begins with all of the possible variables and selectively deletes them based on the specified criteria, which is designed to minimize prediction bias. This continues until a chosen threshold level is exceeded. A threshold, or "delta" is chosen to be smaller if the desired accuracy is to be better. The 'step-up' method is the opposite. It starts with no variables and selectively adds them until a threshold is reached. This procedure uses criteria for selection that are designed to minimize prediction error.

Measurements of standard error of prediction (SEP) are used to compare one wavelength set with another and are also compared to the result with no selection. Before wavelength selection, both validation and calibration data sets are Fourier bandpass filtered using a Gaussian window.

One of the wavelength selection routines is then used on the calibration data. The results are used for both calibration and validation. Once the wavelengths have been selected, a calibration PLS model is built and then validated. The standard error of prediction (SEP) is then calculated for the validation data set. Each of the four wavelength selection routines centered around the same region of 2.24 to 2.33 μm . It was found that as little as eleven of the original 618 wavelengths could be used to predict glucose concentration to the same SEP as using all the wavelengths.

These results are highly significant for this study which focuses on the miniaturization of a final sensor. By reducing the number of wavelengths by nearly two orders of magnitude to 11, we can realize a sensor based on a series of monochromatic light sources such as laser diodes to potentially be used in place of the current FTIR bench top system. This has huge advantages for space flight including lower power consumption, lighter weight, smaller size, and less cost while maintaining the accuracy of the current FTIR system.

Effect of Sample Temperature and pH:

To further improve the analytical signal collected from the sample, several strategies are being investigated with regard to sample pH and temperature monitoring and control. Experimental results produced elsewhere and confirmed in our lab indicate that pH and temperature affect the position of water absorbance bands. These must be controlled or accounted for in any absorption-based instrument. We have investigated and are continuing to investigate these ideas.

Water has been shown to have profound effects on spectral characteristics of many species. Sugars and amino acids such as alanine, in particular, exhibit sharp spectral features in crystalline form, but these are broadened when dissolved in aqueous solution.² (Reeves, 1993). The positions of glucose absorbance peaks do not change with temperature or pH, but those of the underlying water bands do. We are interested in monitoring and correcting the temperature and pH effects on the water absorbance profiles.

When considering the spectral subtraction necessary to extract spectral information about glucose, these shifts cause large baseline and slope variations in the data. While these problems can be eliminated through data preprocessing techniques such as digital filtering, a potential advantage can be realized through more direct monitoring and control of temperature and pH that affect the water baseline.

A three-part study is currently underway on the effects of pH and temperature on the spectra of cell culture media. First, the separate effects of pH and temperature will be determined. Second, an investigation of the combined effects will be undertaken to determine any coupling between the two. We intend to pursue these studies in order to establish the exact role of pH and temperature on the glucose concentration prediction. The software will be

II. MSAD Program Tasks — Ground-based Research

Discipline: Biotechnology

appropriately modified to account for any necessary corrections for temperature and pH variations. A temperature sensor (a microthermocouple) and pH meter could be incorporated in the final system if these effects are proven to have a significant role in the prediction routines.

References:

1. Brown PJ, Spiegelman CH, and Denham MC, "Chemometrics and spectral frequency selection," Phil. Trans. R. Soc. Lond. A, vol. 337, pp. 311-322 (1991)
2. Reeves JB, "Influence of Water on Near-Infrared Spectra of Model Compounds," Jour. of AOAC Int., vol. 76, No. 4, pp. 741-748 (1993)

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 2
PhD Students: 1

TASK INITIATION: 9/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-23-01-36

NASA CONTRACT No.: NAG9-821

RESPONSIBLE CENTER: JSC

A Comprehensive Investigation of Macromolecular Transport During Protein Crystallization

PRINCIPAL INVESTIGATOR: Dr. Lawrence J. DeLucas

University of Alabama, Birmingham

CO-INVESTIGATORS:

Chait, A.
Meyer, W.

NASA Lewis Research Center (LeRC)
NASA Lewis Research Center (LeRC)

Task Objective:

The objective of this program is the collection and data analysis of protein crystal nucleation events and the development of theoretical mechanisms to support experimental molecular transport conditions for growing crystals.

Task Description:

The proposed research represents a multi-disciplinary effort to develop a realistic model based on observed and modeled behavior of macromolecular transport during protein crystallization is a diffusion dominated regime. Two phases of this project were described in the original proposal. The first phase involved developing a ground-based system from which comparative studies between crystal growth in solution versus crystal growth in a gel medium (with reduced convection) could be performed. The second phase represents a transition from ground-based research to the development of a space-based hardware system that further expands the techniques and lessons learned from the ground-based work. Thus, in year one and in subsequent years, this proposal will concentrate primarily on the ground-based research.

Task Significance:

These studies should provide the basis for rational optimization of equipment and process parameters (e.g., initial supersaturation and rate of change of supersaturation) for Earth-based crystal growth. The combination of diagnostics and modeling will allow the critical examination of various hypotheses emerging in the literature. In the long term, these studies will address differences between transport mechanisms on Earth and in space.

Progress During FY 1996:

"An Investigation of Protein Crystal Growth by Laser Light Scattering"

The goal of this work is to detect and monitor the macromolecular events leading to the nucleation of protein crystals by probing the growth solution in a non-invasive way, via Dynamic Light Scattering (DLS). Two proteins, lysozyme and protamine insulin, were studied. Crystallization was induced in both cases by using temperature as a dynamic parameter. The light scattering experiments with lysozyme indicated that low protein, high ionic strength solutions showed a large increase in effective hydrodynamic radius as well as an increase in forward scattering. Any resulting precipitate was amorphous or amorphous with orthorhombic crystals. These solutions showed a rather slight increase in hydrodynamic radius, and sometimes in forward scattering, during nucleation. After crystals were visible, the hydrodynamic radius reached a maximum, and finally decreased to near the initial value. DLS experiments with insulin gave inconsistent results. Only the onset of the "active period" during which bright scintillation appeared in the scattering volume could be detected, although this event also made DLS measurements difficult. This active period always precede the appearance of crystals. For insulin crystallization, light scattering proved to be an effective detector of nucleation but analysis of the phenomena occurring during nucleation remained elusive. Results from this project confirm that laser light scattering can be effectively used as a monitor of the nucleation of relatively small proteins. They also demonstrate that the presence of higher order aggregates in solution is not necessary for nucleation.

"Rotational Protein Crystal Growth Device and Interferometric monitoring of Protein Crystal Growth in Gel"

This project encompasses two studies: (1) the growth of a protein crystal free-falling in an up-flow solution, and (2) the detection of nucleation and growth of lysozyme crystals in Agarose gel medium with optical and interferometric methods. The first study found that both static contact of the crystal with a surface and the

sedimentation of the crystals were eliminated. Inhomogeneities in the supply of nutrient were also severely reduced. The effectiveness of this growth method appears dependent upon the type and purity of the protein, and is mainly limited by the consequences of mechanical action on the protein solution. The second study used interferometry to monitor temperature controlled crystal growth in gels, where gravity induced convection flows were reduced. Information about the transport of nutrient around the crystal as well as the protein aggregation process were correlated with protein crystal quality. The results indicate that gel growth has the potential to produce high quality protein crystals, but remains limited in application because of the small amount of data available for the temperature dependence of protein solubility.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 9/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-23-08-35

NASA CONTRACT No.: NAG8-116

RESPONSIBLE CENTER: MSFC

Development of Robotic Techniques for Microgravity Protein Crystal Growth

PRINCIPAL INVESTIGATOR: Dr. Lawrence J. DeLucas

University of Alabama, Birmingham

CO-INVESTIGATORS:

Torre, L.

Boeing Aerospace

Tillotson, B.

Boeing Aerospace

Task Objective:

The main objective of this work is to eventually develop advanced capabilities which will enable the next generation of microgravity protein crystal growth (PCG) research facilities to grow and identify superior crystals for crystallographic research. Machine vision and PCG-specific imaging modes will be used to provide feed-back for improved dynamic control of the crystal growth process. Similar technologies will be used to automate the visual evaluation of crystals. New methods for manipulating fragile crystals and for controlling protein concentration will be evaluated as a means to improve the crystal growth process. These enhanced research capabilities will then be transitioned into payloads for the space shuttle and, ultimately, the international space station. It is believed that these capabilities will also directly benefit ground-based investigations in academia and industry.

Task Description:

A multi-disciplinary approach which combines engineering, robotics, optics and crystallography has been initiated. Non-invasive methods for manipulating crystals in low gravity have been investigated in year one of this proposal. Machine vision and optical techniques have also begun to be developed and will eventually be applied to evaluate the size and quality of crystals, both to select crystals for x-ray analysis and to guide the optimization of initial growth conditions.

Task Significance:

Successful completion of this program should result in an increased yield of large, high quality crystals for macromolecular crystal growth experiments, particularly in microgravity, and to enhance crystallographers' ability to evaluate macromolecular crystals stability for x-ray analysis.

Progress During FY 1996:

In the original proposal, we outlined a four-year approach in which we would evaluate systems and methods for achieving each of our objectives in the ground-base research during the first two years. The second and third years would be used to refine the most promising methods and develop a conceptual design for their incorporation into future flight experiments. Assuming successful science readiness reviews in the third year, we anticipate flying crystallization experiments during years three and four in a microgravity environment to produce higher quality crystals and to demonstrate automated selection of high quality crystals. Finally, during the fourth year we anticipate finishing post-flight data reduction and submitting articles for publication and final reports for NASA. A close coordination between the principal investigator, Dr. Larry DeLucas, and the science team has been developed with scientists and engineers from the Boeing Defense and Space Group in Huntsville, Alabama.

The following summarizes the tasks accomplished during the last fiscal year:

- (1) Defined a basic concept for a shuttle experiment to test the utility of diamagnetic manipulation for improved growth of protein crystals in microgravity.
- (2) Defined and carried out reduced gravity experiments that verify the ability of the proposed experiment concept to passively control the position of protein crystals.
- (3) Defined and carried out reduced gravity experiments that verify the principle of magneto-chemical convection in fluids that are somewhat representative of protein crystal growth solutions.
- (4) In cooperation with NASA Lewis Research Center, defined an experiment to determine whether magnetic fields

have a noticeable effect on the ability of protein solutions to form crystals. Results have been computed, but refinement of the model is still underway.

(5) Defined an experiment to determine whether magnetic fields have a noticeable effect on ability of protein solutions to form crystals. The experiment started very recently, so no definitive results are yet available. This work should refine preliminary experiments funded as Boeing Independent Research and Development in CY 1994, which verified that lysozyme crystals would grow in the presence of substantial magnetic fields. However, the 1994 experiments were not well documented nor were the crystals subject to expert evaluation.

(6) Conducted preliminary PCG experiments in which manganese chloride was substituted for sodium chloride in preparation of the growth solution. These experiments verified that protein crystals can be grown in solutions whose magnetic properties have been tailored to enhance magnetochemical convection and magnetic control of crystal position.

(7) Attempted to measure the magnetic susceptibility of various components of PCG solutions.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 9/95 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 962-23-08-36

NASA CONTRACT NO.: NAG8-114

RESPONSIBLE CENTER: MSFC

Macromolecular Crystallization: Physical Principles, Passive Devices, and Optimal Protocols

PRINCIPAL INVESTIGATOR: Dr. George T. DeTitta

Hauptman-Woodward Medical Research Institute

CO-INVESTIGATORS:

Luft, J.R.

Hauptman-Woodward Medical Research Institute

Task Objective:

The objective of our work is to design, test, and evaluate devices and protocols for growing single crystals of macromolecules suitable for x-ray diffraction experimentation. In the process we propose to identify those devices and protocols that will work optimally on earth, and to identify those that may benefit from a microgravity environment. Our objective is to quantitatively assess those parameters that have a profound effect on crystal quality.

Task Description:

The work centers on a fundamental understanding of the role of kinetics in determining the ultimate quality of macromolecular crystals grown in the 1-g laboratory. Our preliminary work was to propose and fabricate a number of prototype devices that can work to control the kinetics of equilibration in vapor diffusion crystallization experiments. Our present work is to understand the basic processes that underlie the vapor diffusion process, and to confirm the assertion that the rate-limiting step in vapor diffusion is transit of water across the vapor space.

Task Significance:

Macromolecular crystallography has become the foundation stone of much of modern biology. Protein engineering, molecular genetics, and rational drug design depend on an accurate description of the structure of a macromolecule (typically a protein) at the atomic level. Such a view is afforded by few disciplines, and the principal one is crystallography. A necessary first step in structure determination is the growth of a single crystal suitable for diffraction studies. Our work is aimed at a greater understanding of the processes of crystal growth, and at the design and testing of devices and protocols to grow better macromolecular crystals. Modern approaches to drug design rely on an accurate understanding of the target molecules of drugs and therefore our work has the potential to materially affect the general public who will benefit from new drugs that result from these approaches.

Progress During FY 1996:

Testing and development of methods and devices designed to passively control vapor phase equilibration in protein crystallization experiments continued. A protocol using reservoir volume rather than concentration to screen micro-endpoint equilibration is being developed. This method will reduce cost of setups and may improve crystal quality through reduction in endpoint dehydration rates with an asymptotic approach to equilibration between the protein and "reservoir" droplets. Thermal gradient batch methods are under development. Temperature is used to control the level of supersaturation of the macromolecule under a variety of chemical conditions using a macro (200 microliter) and micro (5 microliter) capillary batch technique.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/95 EXPIRATION: 7/99

PROJECT IDENTIFICATION: 962-23-08-41

NASA CONTRACT NO.: NAG8-115

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Luft, J.R., Albright, D.T., Baird, J.K., and DeTitta, G.T. The Rate of Water Equilibration in Vapor-Diffusion Crystallizations: Dependence on the Distance from the Droplet to the Reservoir. *Acta Crystallographica*, vol. D52, 1098-1106 (1996).

Presentations

DeTitta, G.T. "Preliminary Evaluation of Thermal Gradients as Tools for Macromolecular Crystal Growth." Recent Advances in Macromolecular Crystallization, LeBiscenbourg, France, June 2-4, 1996.

DeTitta, G.T. "HOT and COLD: The Story of Three Thermal Gradients in Search of the Perfect Crystal." Protein Crystal Growth Conference, Panama City Beach, Florida, April 28-30, 1996.

DeTitta, G.T., Dembik, D.M., Pangborn, W.A., and Luft, J.R. "Polythermal Screening and Production Methods for Macromolecular Crystallization." International Union of Crystallography XVII Congress and General Assembly, Seattle, Washington, August 8-17, 1996.

The Effect of Microgravity on the Human Skin Equivalent

PRINCIPAL INVESTIGATOR: Dr. S. D. Dimitrijevic

Univ. of N. Texas Health Science Ctr, Fort Worth

CO-INVESTIGATORS:

Mills, D.O.

University of North Texas Health Science Center @ Fort Worth

Task Objective:

The objective of this project in the first instance is to effect morphogenesis of The Human Skin Equivalent under the conditions of simulated microgravity and compare its tissue characteristic properties with those of the Skin Equivalent generated under 1g conditions. We will then study the effects of fluctuating levels in several physiological parameters (e.g., glucose and calcium), which intact organisms experience under zero gravity, on the development and functions of our *in vitro* model of human skin.

Task Description:

We have developed several living *in vitro* models of human tissue (e.g., skin, cornea, conjunctiva), based on a non-contracting three-dimensional collagenous matrix populated with appropriate fibroblasts. Because these models support functional epithelia and/or endothelia and closely mimic *ex vivo* human tissue, they provide an excellent opportunity for studies of cell-cell and cell-matrix interactions during tissue development or repair. Of equal importance are the responses of these models to changes in their microenvironment and return to the quiescent state. We will, therefore, examine all stages of development of the skin equivalent ranging from fibroblast behavior and function, attachment of keratinocytes and melanocytes, and epidermopoiesis under the conditions of simulated microgravity. We also intend to study the effect of changes in glucose and calcium homeostasis, transiently occurring under zero gravity in man, on the Human Skin Equivalent cultured in RWV. Finally, we propose to determine if the exposure of tissue to simulated microgravity represents a stress to which cellular components respond by expression of stress proteins.

Task Significance:

Simulation of the microgravity environment using RWV has been found to be a unique environment in which cells which are otherwise difficult to grow may be successfully cultured. Furthermore, under these conditions, a number of cells form large aggregates. We hope to demonstrate that the simulated microgravity environment is also conducive to generation of human tissue, and that such tissue will possess biological and mechanical integrity appropriate for use in tissue replacement therapy. We further hope to increase our understanding of tissue tolerance to the transient physiological abnormalities experienced under zero gravity, and enhance our understanding of how these might impact tissue development and repair and contribute to the design of new approaches to wound healing.

Progress During FY 1996:Background

Our interest in cell-matrix interactions has led to the development of three-dimensional models based on non-contracted collagen type I gels inhabited by fibroblasts derived from normal human tissues. Cells populating such gels are ideally situated for gravity nullification because the "high viscosity" of the matrix restricts the centrifugal acceleration generated in the rotating-wall vessel (RWV). Thus rotation of the developing tissue around a horizontal axis at a constant angular velocity allows each component of the living system to describe a perfect circular path independent of rotational speed (Stokers' motion).

Modified Rotating-Wall Vessels (RWVs)

Initially, human skin equivalent (SE) construction requires polymerization of collagen type I solution containing normal dermal human fibroblasts into a three-dimensional gel-dermal equivalent (DE). After fibroblasts have adapted to the matrix, keratinocytes (alone or mixed with melanocytes) are plated on the surface of the DE and allowed to attach and form a confluent monolayer. Differentiation of keratinocytes into a stratified cornified epidermis is then effected by raising extracellular calcium and elevation of the SE to an air-liquid interface.

Our early experiments showed that the vessel cylinder wall is too highly polished and hydrophobic to allow polymerization of collagen into a three-dimensional gel matrix. Consequently, during the past year, we have

II. MSAD Program Tasks — Ground-based Research

designed and evaluated two RWV formats, based on the 50 ml STL V, which satisfy our gravity nullification requirements and are suitable for the construction of the SE. One modification (M1) involved machining four segmental compartments into the rear end cap of the STL V; the other modification (M2) has four identical size compartments machined into the vessel cylinder. In M1, DEs are cast simultaneously in the four compartments (generating segments of tissue), whereas in M2, DEs are cast in each compartment individually to produce rectangular pieces of tissue. Using either vessel, one RWV culture set up is used to generate four DE/SE under identical conditions. Since the experimental protocols involved in SE development require a minimum of 3 weeks, our modified RWVs also optimize hardware utilization.

Dermal Equivalents Generated in RWV

Fibroblast Phenotype: We have shown that the weight, volume, and therefore, density of DEs generated in 1g are independent of collagen type I concentration (3-5mg/ml) and cell number (fibroblasts, 10^5 - 5×10^5 cells/ml). Under these conditions, there is also no significant cell division or migration. This *in vivo*-like quiescence is maintained in the DE generated under microgravity during a 15-day observation period. Since fibroblasts respond to mechanical stimuli and are responsible for tissue contraction, developing DE is very sensitive to mechanical stresses. It was particularly important to observe that DEs generated in the RWV do not contract. In addition to indicating an absence of the "activated" fibroblast phenotype, the myofibroblast, this finding also suggests that the microgravity environment does not appear to impose significant mechanical stress on the DE.

Treatment of the DE with neutral red confirmed cell viability. Paraffin-embedded, cross-sectioned DE showed a random distribution of cells throughout the matrix. In contrast, some "sedimentation" for fibroblasts is frequently observed under 1g conditions.

Confocal microscopy: A more detailed and precise assessment of fibroblast distribution, orientation, and interaction with the collagen matrix will be obtained from studies of DEs by confocal microscopy (CFM). In order to facilitate such findings, we have developed methods for labeling fibroblasts with fluorescent Cell Tracker dyes, and incorporated the labeled viable cells into DEs. The utility of this technique was demonstrated by the analysis of orientation of a single fibroblast in a DE, which was defined by eight optical sections obtained at 9m intervals. Cell-matrix interactions are highly dependent on cell surface matrix receptors (integrins) and the extracellular components present. We are currently studying the expression of collagen-specific integrins and the organization of collagen fibers in DEs developed in the RWV.

Mechanical Properties: Tensile strength of skin, primarily a feature of the dermis, is particularly important in the context of wound healing and clinical use of SEs as graft tissue. Preliminary experiments suggest that DEs generated in the RWV have a lower tangential stiffness (about 3-6 fold) than normal human dermis. Such differences in mechanical properties might be expected in view of the lower collagen fiber density in DE as shown by transmission electron microscopy.

Metabolic Activity: Cell viability in DEs cultured in 1g can be maintained for the period of time required for epidermalization of the SE. Preliminary morphological data obtained from RWV experiments suggests that fibroblasts begin to show signs of distress after about 2 weeks. Initial metabolic studies suggest that glucose depletion or lactate accumulation are probably not contributing stress factors. Since the DE is submerged under a considerable volume of medium, hypoxic conditions might develop. Increasing oxygenation of the DE will be discussed below.

Skin Equivalents Generated in RWV

Construction: Although normal human keratinocytes and melanocytes are readily available in our laboratories, the initial focus is on the effect of microgravity on bicellular SE composed of fibroblasts and keratinocytes. Conditions for growth and differentiation of keratinocytes, which are also optimal for melanocyte survival, are being developed to facilitate the construction and studies of the tricellular SE.

In a typical SE construction experiment, once DEs are established, the medium (Hams F12) is removed from the RWV, keratinocytes are placed on and allowed to attach to the surface of DEs (2-3 hours). The vessel is then charged with keratinocyte growth medium (KGM) and set to rotate. When the keratinocyte monolayer is confluent, differentiation is initiated by raising the extracellular calcium. Such developing SEs, when paraffin embedded and cross-sectioned, show that differentiation through several suprabasal layers (including the granular layer) does take

place. The lack of cornification, however, suggests that for complete maturation, the SE needs to be cultured at an air-liquid interface (sufficient oxygen). This is consistent with our earlier work which showed that epidermalization of the SE is stimulated by exposure to hyperbaric oxygen.

A stronger attachment of keratinocytes to the DE observed under RWV conditions indicates increased adhesion. This is manifested by increased tissue integrity at the dermal-epidermal junction observed during sectioning of embedded SEs. Expression of adhesion molecules by keratinocytes and melanocytes under microgravity is presently under study.

SE Vessel: In order to provide conditions which will allow exposure of the SE surface to air and improve oxygenation and nutrition of the DE, we have developed a third format of the RWV. In this modification (M3), the vessel is composed of two parts, each of which has its own diffuser and medium exchange parts. the "vessel divider" is composed of two discs, each containing six wells, which sandwich a semipermeable membrane. The membrane forms the "floor" of each of the six wells, providing each well with an apical and a basal side. DEs are cast in the wells and the oxygenation and nutrients are supplied from both sides. Furthermore, SEs in the wells are at the air-liquid interface when one of the vessel changers is operated with very little or no medium. We are currently evaluating this vessel format, and preliminary experiments suggest that it will satisfy the required criteria.

Confocal Microscopy of the SE: We believe that confocal microscopy will be a useful tool for studying processes involving cell-cell and cell-matrix interactions in the SEs as well as the DE. Consequently, we have shown that keratinocytes and melanocytes may be prelabeled with fluorescent Cell Tracker dyes. The fluorescence is retained in the cells through cell harvesting, seeding on DEs, proliferation, and differentiation. The SE labeled in this manner can be fixed, paraffin embedded, sectioned, and the cross-sections deparaffinized with retention of fluorescent label. Initially, this methodology will lead to the development of attachment and proliferation assays.

Technology Transfer

From the inception of this project, we have worked closely with Synthecon, Inc. Their experience in engineering and manufacturing of RWVs was instrumental in generating vessels suitable for our specific tissue assembly requirements. Prototypes of M1 and M2 were displayed at the Houston Investigators Working Group meeting earlier this year. An agreement is in place for the exclusive manufacture of the modified vessels, and these should eventually be available for general use.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 9/95 EXPIRATION: 8/99
PROJECT IDENTIFICATION: 962-23-01-37
NASA CONTRACT No.: NAG9-813
RESPONSIBLE CENTER: JSC

Use of Microgravity-Based Bioreactors to Study Intercellular Communication in Airway Cells

PRINCIPAL INVESTIGATOR: Dr. Ellen R. Dirksen

University of California, Los Angeles

CO-INVESTIGATORS:

Woodruff, M.
Biotano, S.

UCLA School of Medicine
UCLA School of Medicine

Task Objective:

1. To develop protocols for optimal culturing of airway epithelial tissue in low shear stress simulated microgravity, rotating-wall zero-headspace vessels (RWV).
2. To measure the ability of airway tissues cultured in simulated microgravity to communicate intercellularly.
3. To measure and characterize mechanically-sensitive ion channels in the plasma membranes of isolated cells grown in low shear stress microgravity simulating RWV.

Task Description:

We have been studying a cell calcium signaling mechanism in our laboratory that is expressed in a wide range of tissues and that may be used to help evaluate normal cell and tissue functional integrity. We have characterized a mechanosensitive change in intracellular calcium concentration ($[Ca^{2+}]_i$) in an individual cell that is communicated over a large area of the cultured epithelial tissue by gap junctional-mediated diffusion. We have developed precise and accurate techniques for observing the cellular Ca^{2+} changes in an array of cells in real-time using a computer based video imaging system. This has allowed us to implicate particular components of the signal transduction pathway, including mechanosensitive release of effector molecules (e.g., inositol 1,4,5-trisphosphate and Ca^{2+}), and membrane ion channels (Ca^{2+} -conductance channels). We have recently discovered that interference with signaling has a long-term effect on cell migratory behavior, and we are also exploring the possibility that mechanosensitivity relies on the function of the cytoskeleton. We will carry out the task objectives as described above. The experiments that we are proposing will assay the effect of Earth-based, simulated microgravity on the intercellular communication of the mechanically-induced Ca^{2+} signal and on the expression and control of mechanosensitive cation-specific and Ca^{2+} channels that are related to signaling. Cells will be grown in an RWV and then characterized for 1) whole tissue growth characteristics such as aggregation, morphological differentiation, viability and tissue growth, 2) second messenger signaling such as mechanosensitivity, magnitude of $[Ca^{2+}]_i$ increases and intercellularly communicated Ca^{2+} responses, and 3) channel activity including single ion channel currents and whole-cell mechanosensitive ion channel currents. We will use as controls cells cultured in parallel at unit gravity in organ and tissue cultures.

Task Significance:

Intercellular communication is essential for coordinated cellular activity and proper tissue response. It is presently unknown whether tissues produced under microgravity conditions have intercellular communication. In contrast, cells grown under conditions where the effect of gravity is randomized might demonstrate a potentiation of intercellular communication.

Airway epithelial cells, as they are presently cultured, have several limitations. The morphology of cells in monolayer cultures, unlike those in the intact epithelium, take on an amorphous, flattened shape, and the percentage of ciliated cells is markedly reduced as cells migrate away from the explant. Cells do not stay attached to the collagen substrate for more than 2 to 3 weeks in culture and therefore do not survive for an extended time, limiting our ability to examine the long-term effects of agents that are added extracellularly and intracellularly. This is a serious limitation since we would like to study biomolecules that control differentiation and maintenance of the cells and relate this effect to the expression and elaboration of gap junctional communication. Microgravity has been shown to extend the lifetime of cultures of a number of tissues and may also produce this beneficial effect in airway epithelia. It has been suggested that microgravity-based culture systems may have great potential for medical science in the area of tissue engineering. The success of this hypothesis is dependent on developing fully

functional tissues under microgravity conditions. Our proposed research will elucidate cell-cell interaction mechanisms that are sensitive to gravitational forces. These results will lead to information for improving tissue growth so that the full potential of biological systems under microgravity can be realized.

Progress During FY 1996:

Culture of airway cells and tissues for simulated microgravity studies: Our efforts have focused on developing a method of culturing airway epithelial cells in the simulated microgravity environment of the RWV to facilitate the study of the cells by light microscopy, calcium imaging, and electrophysiology techniques. Primary cultures of airway epithelial cells in the randomized simulated microgravity of the RWV were initially difficult to establish. We used collagen-coated microcarriers to provide the required substrate for anchorage-dependent airway epithelial cells while promoting cell attachment and growth. The initial problem of sparse attachment of cells to beads was overcome by adjusting the seeding density, allowing for settling periods, and treating the beads with fetal bovine serum and fibronectin to promote cell adhesion. Early viability was improved by designing a gentle, 18-hour, low enzyme concentration method for cell dissociation. Different culture media, FBS concentrations, and serum-free growth factor combinations were evaluated until a regimen was developed which fostered proliferation of cells. The culture conditions promoted growth of airway epithelial cells in layers covering the microbeads and sustained epithelial cells for 3 weeks. By immunocytochemical anti-cytokeratin staining, the majority of the cells were identified as epithelial, with occasional ciliated epithelial cells and some fibroblasts. The only difference between cells on microbeads, placed upon a coverslip to serve as a unit gravity control, and suspended cells on microbeads in the RWV was that the cell layer often did not cover the cap of the microbead at unit gravity. Although the thin layer of cells on translucent collage-coated microbeads permitted observation by light microscopy, examining several cells at one time was difficult because all the cells in a spherical monolayer were at different planes of focus. Cells had to be removed from the microbeads to enable our observation of multicellular interactions.

At present, intact airway epithelium is being cultured as small explants at unit gravity and under simulated microgravity conditions in a form most similar to its native, *in vivo*, state. Small (less than 1 mm²) pieces of airway mucosa are grown in suspension in the RWV and in organ culture at unit gravity. The RWV culture maintains the differentiated phenotype and survival of airway epithelial cells for a least two weeks. The RWV cultures appear to be an improvement over unit gravity organ cultures in which we have routinely maintained healthy tissue for only one week. Since the intact airway epithelial pieces are opaque to standard light microscopy, we are developing protocols for the recently purchased Zeiss confocal laser scanning microscope to measure intercellularly communicated changes in [Ca²⁺]_i, using the Ca²⁺ dye fluo-3. In our preliminary studies, intact airway epithelium responds to the agonist ATP with an increase in [Ca²⁺]_i. Currently, we are continuing our work to improve tissue maintenance in the simulated microgravity environment and to study the role microgravity plays in how cells sense and respond to mechanical stimuli.

Confocal laser scanning microscopy (LSM) of whole epithelial explants: Intact tracheal epithelial layers were microdissected from rabbit tracheas, cut into 0.5 - 1.0 mm² explants, and suspended in culture medium. Half of the tissue was seeded in untreated culture dishes (designed for suspension culture) for culture at unit gravity. A rotating-wall vessel was inoculated with the remaining tissue for culture in simulated microgravity. Cells maintained the columnar morphology and pseudostratified architecture characteristic of tracheal epithelium *in vivo*, over 1 week in culture, with no apparent difference between cells maintained at unit gravity versus simulated microgravity environments. Confocal fluo-3 imaging was used to evaluate mechanically-induced intercellular Ca²⁺ communication in intact tracheal epithelial explants after 5-7 days in culture. Explants are incubated in fluo-3 AM, a calcium indicator dye, and settled on Cell-Tak-coated coverslips. A Zeiss LSM was used to measure changes in fluo-3 fluorescence in a 3 mm thick optical cross-section through the tissue. Using this technology, we have been the first to observe Ca²⁺ responses in intact tracheal epithelium. Cells from both unit and microgravity cultures displayed robust increases in ([Ca²⁺]_i), as reflected by increased in fluo-3 fluorescence, in response to agonist-stimulation with 50 mM ATP. When a single cell in the epithelium was touched with a microprobe, we observed a Ca²⁺ wave in which fluo-3 fluorescence increased first in the mechanically stimulated cell (56 ± 9 grayscale values, n = 15), then was propagated after a brief delay to adjoining cells (2.8 ± 0.4 cells from stimulated cell, on each side, n = 15). In comparing Ca²⁺ responses in tissue maintained in simulated microgravity with those maintained at unit gravity, no significant difference was found in the average number of cells involved in a Ca²⁺ wave, the magnitude of the increases in fluo-3 fluorescence, the time cells required for recovering resting Ca²⁺ after

mechanical stimulation, or in the speed of wave propagation. Preliminary results indicate that intercellular Ca^{2+} communication changes over time in culture and we are currently investigating this in more detail.

Fura-2 fluorescence imaging of enzymatically dissociated cells: In our proposal, we outlined a procedure to evaluate whether cultures of epithelium grown under microgravity conditions could maintain the ability to communicate intercellular signals through gap junctional communication. Both microgravity- and unit gravity-grown cells were to be monitored for their ability to communicate Ca^{2+} signals from cell to cell after localized stimulation of a single cell by micropipette.

Ca^{2+} signaling in microgravity-grown epithelial cultures. Cells grown on collagen-coated microbeads, under simulated microgravity conditions as described above, were digested by pronase (1% in HBSS for 10, 20 and 30 min.). This produced largely single cells. These cells were then allowed to settle onto con A-coated glass coverslips and were loaded with 5 mM fura-2-AM dye for one hour. Cells isolated in this manner responded to mechanical stimulation and ATP addition by increasing their intracellular Ca^{2+} concentration ($n = > 40$ cells in 4 expts). Therefore, microgravity did not significantly alter the ability of epithelial cells to respond to external stimuli with changes in $[\text{Ca}^{2+}]_i$.

Ca^{2+} signaling in dissociated cells obtained from explants. Tracheal explants, similar to the tissue used for the confocal studies, are maintained for up to a week as controls and under microgravity conditions in the rotating-wall vessel. These explants are treated with pronase (0.5% in HBSS for 10 min. at 37°C , resulting in cell clusters. Clusters are then subjected to a series of gentle centrifugations and resuspensions in fura-2AM supplemented HBSS (5 μM , 10 min., two resuspensions) and HBSS (10 min., two resuspensions) alone. After a final centrifugation in HBSS, the solution is aspirated to 0.75 ml, and the remaining cell solution is gently agitated and transferred to 18 mm poly-L-lysine coated glass coverslips for analysis of $[\text{Ca}^{2+}]_i$. Centrifugation and resuspension allows for removal of pronase to stop digestion and for fura-2 loading. After a 20 min. incubation on a slide, cell debris is washed away and those cells remain that stick to the coverslip. Single cells within a cluster of at least 3 cells and up to 12 cells are mechanically stimulated and monitored for propagation of Ca^{2+} signals between cells and for full recovery of $[\text{Ca}^{2+}]_i$ of the stimulated cell. We conclude that enzymatically dissociated cells obtained from explants maintained at unit gravity, as controls ($n = 3$) and under simulated microgravity conditions in the rotating-wall vessel ($n = 4$) are capable of intercellular communication as identified by the propagation of mechanically-induced Ca^{2+} waves.

Electrophysiology experiments: In patch clamp experiments, we were able to record from several types of ion channels in enzymatically dissociated ciliated epithelial cells from cultures maintained under microgravity conditions. The purpose of these experiments was to characterize mechanosensitive channel behavior in order to assess if the simulated microgravity environment has any effect on the number or properties of ion channels. The percentage of ciliated cells obtained from the cultured explants maintained under microgravity conditions and the cultures from the same tissue incubated at unit gravity declined with time in culture. Immediately upon dissection of the tracheal mucosa, about 30% of the cells obtained after pronase enzymatic digestion were ciliated. After 4 days of culture, this decreased to less than 1%. In 16 experiments (8 controls and 8 experimentals), we recorded from 4 patches in the cells grown under microgravity conditions and found one channel type in the microgravity-grown cells that appears to be mechanosensitive. Two of the patches contained this channel. This channel has a chord conductance of about 40 pS and a reversal potential near 0 mV. In inside-out patches and in symmetrical solutions the reversal potential was exactly 0 mV. Exposing the cytoplasmic face of the membrane to a solution containing 50 mM K^+ , 85 mM Na^+ (outside face is 5 mM K^+ and 138 mM Na^+) shifted the reversal potential to -10 mV, suggesting that this is a non-selective cation channel with a slightly higher permeability to Na^+ than to K^+ ions. Negative pressure applied to the recording pipet to mechanically stimulate the channels resulted in an increase in the probability of channel opening. Three other types of channels have also been observed; two have conductances of 30 pS and 60 pS and a third is a fast-flickering channel with a conductance of 80 pS. None of these channels show mechanical sensitivity.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 8/95 EXPIRATION: 7/99

PROJECT IDENTIFICATION: 962-23-01-16

NASA CONTRACT NO.: NAG9-814

RESPONSIBLE CENTER: JSC

Microgravity Thresholds for Anti-Cancer Drug Production on Conifer Cells

PRINCIPAL INVESTIGATOR: Dr. Don J. Durzan

University of California, Davis

CO-INVESTIGATORS:

Falk, R.
Havel, L.
Ventimiglia, F.

University of California, Davis
Agricultural University, Brno, Czech Republic
University of California, Davis

Task Objective:

The objective is to develop a model for anticancer drug production (paclitaxel or Taxol™) under microgravity with highly adaptable conifer cell lines.

Task Description:

Ground-based bioreactor research explores how free and bound taxanes are produced under gravitational stimuli using cell suspension cultures of haploid and diploid cells in *Taxus* sp. First, cells from taxane-producing genotypes are evaluated for their growth and drug production in RCCV bioreactors (microgravity), 1 xg, and 3 xg. Second, the yields of free and bound taxanes are determined by a competitive inhibition enzyme immunoassay (CIEIA). Taxanes are recovered by solvent extraction, and quantitated by high performance liquid chromatography. Antibodies to specific taxanes are used to localize sites of biosynthesis on the surface of cells. Bound taxanes are enzymatically removed after solvent extraction of free taxanes. Third, enzymatic surfaces producing bound taxanes are localized by antibodies to portions of the paclitaxel molecule. Laser confocal microscopy for fluorescent-tagged antibody location and scanning electron microscopy with immunological localization of taxanes provide fixed position information for understanding final drug production. Fourth, cells are monitored for markers for programmed cell death (apoptosis) so that drug production can be sustained or even overproduced when linked to gravitational forces.

Task Significance:

Paclitaxel or Taxol™ is a revolutionary natural anti-cancer drug from conifer cells that is effective against ovarian, lung, and breast cancer. The current estimated market for paclitaxel is \$1 billion annually. Paclitaxel also shows promise for the treatment of polycystic kidney disease, for inhibiting angiogenesis in pernicious diseases, and for preventing rheumatoid arthritis and certain diseases of the eye. The many steps and complex chiral structure make total synthesis of paclitaxel commercially impractical. The 'natural' drug is nevertheless preferred to a synthetic product. With bioreactors, the production and recovery of natural drugs are evaluated and controlled under aseptic conditions as cells adapt to gravitational stimuli. Other taxanes produced by cells are identified as substrates to enhance natural synthesis. By contrast, tree farming, harvesting, and processing, while slow, still have to benefit from domestication and tree improvement. Taken together, all approaches are needed to ease the current demand for natural paclitaxel.

A scientific model is needed to predict how cells produce paclitaxel under gravitationally controlled conditions. Process controls that optimize drug recovery as a function of gravity must be identified. In general, physiological stresses, aging, and culture medium supplements are known to increase drug production at 1 xg. Drug production induces apoptosis in animal cells, but until recently, apoptosis was not described for plant cells. An understanding of apoptosis will show us how to sustain and possibly overproduce paclitaxel and taxane in plant-cell bioreactors.

Our cell lines and technologies are protected as intellectual property for use by industry. This study provides an opportunity to test and develop a bioproduct recovery system for plant cell and space-related industries.

Progress During FY 1996:

Two new models for taxane production were established. One postulates how bound precursors are aligned and produced on the cell surface for the final assembly of paclitaxel. The model is based on gravisensing touch genes (*TCH*) that encode calmodulin in signal transduction paths, and on endoxyloglucan transferases that alter cell walls and bind the drug in response to gravitational forces. Experimental results show that some taxanes are bound to

xylan moieties at the 7-OH position of paclitaxel. Other taxanes and paclitaxel are released into the culture medium as insoluble particles.

The second model (Havel and Durzan 1996a) describes how apoptosis, or programmed cell death in plant cells, is related to cell division and to environmental and gravitational stresses. Control over apoptosis is sought to regulate the terminal cellular differentiation of drug-containing wood and bark. The model provides insight into how cells make natural drugs without inducing apoptosis. Experimental results with microgravity demonstrated that cell cycling and metabolic salvage reactions reduced drug production compared to 1xg or hypergravity. Microgravity was used to scale-up cells before drug production induced by gravitational stresses, terminal differentiation, and exposure to elicitors of apoptosis.

A triple-label assay for localizing taxanes and apoptotic and nonapoptotic nuclei in individual conifer cells was developed (e.g. Havel and Durzan 1996b for double-label assay). On cell walls of *Taxus* sp., separate sites for the phenylisoserine side-chain and of baccatin III (oxetane-bearing taxane ring) were localized by laser confocal microscopy in apoptotic and nonapoptotic cells. Experiments demonstrated how separate biosynthetic pathways contributed positionally to the final assembly of paclitaxel on the outside surface of cells and how metabolites were released into the culture medium. The interdiffusion of sites bearing the two precursors represented the esterification of the taxane ring at the C-13 position. Phenylisoserine-containing moieties were found on particles in the culture medium, inside cells, and adjacent to sites producing baccatin III. A polyclonal antibody for the phenylisoserine side chain, and a monoclonal antibody for the oxetane ring probed the internal and external cell structures. Antibodies for different parts of the paclitaxel molecule have been labeled with different sized gold particles for examination by scanning and transmission electron microscopy for study in the final year of this study.

Protoplasts, produced by enzymatic digestion of cell walls, were assayed by the double-label antibody test for parts of the paclitaxel molecule. The phenylisoserine moiety of paclitaxel was found primarily in transvacuolar strands bearing gravisensing amyloplasts and nuclei (haploid cells are coenocytes). As protoplasts became further digested, the transvacuolar strands collapsed and formed vacuoles. Intense labeling was found around apoptotic nuclei.

Free and covalently bound taxanes were recovered from haploid and diploid cells of several *Taxus* sp. in Synthecon HARV and RCCV bioreactors. The RCCV design was more suitable for long-term culture of conifer cells. Bioreactor design and shape altered the HPLC-recovery pattern of taxanes from cells over 2 weeks at microgravity, 1xg and 2xg. Results indicated the need for greater process controls and identified new parameters for enhancing drug production. An accurate estimate of total drug recovery was not yet feasible because taxanes remained tightly bound to membranes, cellular materials, and to insoluble particles released by cells into the culture medium.

Tracheids were produced by the terminal differentiation of apoptotic diploid cells. The coating of tracheids by taxanes supported the notion that one role of taxanes is to prevent the invasion of microorganisms and fungi that attack the explant-donor trees.

The conditioning of the culture medium by cell clusters produced secondary metabolites similar to those made by the bark of trees. Because of costs, volume, and design limitations of the RCCV bioreactors, another clinostat system at 1 rpm using 1 liter flasks, was built for scale-up chemical and biochemical work. This has increased the capacity of our lab to produce ca. 10 liters of cell suspension under simulated microgravity from 60 rotating flasks. No significant differences ($t_{0.05}$ and 12 df) for drug yield over 14 days was found when nipple flasks were compared to RCCV bioreactors.

Apoptosis was observed in cells with and without detectable free paclitaxel. Apoptotic changes in nuclei were initiated by endonucleases and proteases. The destruction of nuclei was followed in three-dimensions by laser confocal microscopy and related to the subcellular localization of taxanes. As nuclei degenerated, cavities were formed by endonuclease activities before nuclei collapsed. Studies are in progress to show how levels of bound taxanes in individual apoptotic cells are altered by gravitational stress.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 8/95 **EXPIRATION:** 8/99

PROJECT IDENTIFICATION: 962-23-01-28

NASA CONTRACT No.: NAG-9-82

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Havel, L. and Durzan, D. Apoptosis in plants. *Botanica Acta*, 109, 268-277 (1996).

Havel, L. and Durzan, D. Apoptosis during diploid parthenogenesis and early somatic embryogenesis of Norway Spruce. *Intl. J Plant Science*, 157, 8-16 (1996).

Proceedings

Durzan, D., Ventimiglia, F., Falk, R., and Havel, L. "Covalently bound taxanes in yew suspension cultures ." *Cellular and Molecular Biology 42/Congress Suppl.*: 27. Abst. 34, 1996.

Presentations

Durzan, D. "Taxane biosynthesis at the individual cell level." VivoRx Pharmaceuticals, April 23, 1996.

Patents

Patent Approved, U.S. Patent #: 5,547,866 Durzan, D. and Ventimiglia, F. "Taxane production in haploid derived cell cultures."

Laser Scattering Tomography for the Study of Defects in Protein Crystals

PRINCIPAL INVESTIGATOR: Dr. Robert S. Feigelson

Stanford University

CO-INVESTIGATORS:

DeLucas, L.

DeMattei, R.C

University of Alabama, Birmingham (UAB)

Stanford University

Task Objective:

The principal objective of this research program is to apply the laser scattering tomography technique (LST) to the study of defects in protein crystals and how these defects relate to growth conditions and x-ray diffraction performance.

Task Description:

This research effort is designed to provide an in-depth understanding of the nature of the defects present in protein crystals using the fast and non-destructive LST technique. A major component of this program will be a comparison between microgravity-grown and terrestrial-grown crystals to help establish the link between microgravity conditions and the improved crystal quality of space-grown crystals. The program will begin with the design and construction of the LST apparatus. The system will be tested on Lysozyme and used to study at least four other protein systems representative of crystals which have been or are being grown in μ g. Crystals grown in the laboratory will be evaluated along with space-grown crystals. After the LST crystal characterization studies, these same crystals will be sent to the University of Alabama for x-ray performance evaluation.

Task Significance:

This investigation will clarify the relationship between growth conditions and defects in protein crystals. It will lead to both a better understanding of the mechanisms involved in protein crystal growth and an ability to make a rational choice of growth parameters, thereby permitting an improvement in crystal size and diffraction resolution (quality). The LST technique will also provide an important means of pre-screening protein crystals prior to diffraction experiments with a significant savings in manpower and beam time.

Progress During FY 1996:

During the first thirteen months of this program which included FY96, the Laser Scattering Tomograph apparatus for the study of defects in protein crystals was built. This instrument is a computer-based, multi-component system comprised of motion control, image acquisition and processing, laser, and optical sub-systems operating under a custom designed control program. The heart of the instrument is a PC compatible computer with a Pentium processor running at 100 MHz with 12MB of RAM and a 1GB hard drive. Off-line data storage is provided by a Syquest 135MB removable media drive.

The motion control sub-system was obtained from National Aperture. It is based on a nuLogic motion control board mounted in the computer. The rest of the sub-system for moving the crystal consists of a three axis positioner with the motion along the x and z direction controlled by dc motors with encoder feedback. The y direction is controlled manually. This three axis positioner allows the crystal being studied to be centered in the field of the microscope and then scanned in the x and z directions to provide a layer-by-layer three dimensional view of the defects in the crystal. The stage that holds the crystal on the positioner is backlit using a fiber optic light source so that an image of the crystal can be obtained for comparison to the defect images.

The image acquisition and processing sub-system consists of a Sony AVC-D7 black and white camera attached to a EPIX 4MEG model 10 video board. The EPIX board which is mounted in the computer not only provides image acquisition, but also facilitates the post acquisition processing necessary to build up the final image of the defects in the crystal.

The laser sub-system is a polarized 5mw Helium-Neon laser with focusing optics to provide a calculated focus diameter of 20μ which increases in diameter only 5% over the range of $\pm 100\mu$ from the focal point. Both the laser

and the focusing optics are mounted to allow adjustment in the x, y and z directions to align the laser beam with the optical sub-system and the crystal position. The focusing optics are mounted in a tilt stage to ensure that the beam remains parallel to the unfocused laser beam.

The optical sub-system is based on an Olympus 30MBDF microscope module equipped with 5x, 10x and 20x objectives and a video port for camera attachment. The laser and optical sub-systems along with the x-y-z positioner are mounted on a small optical table to ensure their alignment and isolate them from vibration.

The final image is constructed by removing pixels from successive images (in the EPIX board image buffer) taken as the crystal is scanned in the x direction and placing them in the proper relationship in a second image buffer. This x-y slice through the crystal reveals the defects in that layer of the crystal. Moving the crystal in the z direction allows visualization of the defects throughout the crystal. The control of the motion and image processing is provided by the control program utilizing the function libraries which came with both the image processing board and the motion control board. This program consisting of 1200 lines of WATCOM C/C++ code was written by a student who was hired through the High School Outreach Program for science students at the Center for Materials Research.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/95 EXPIRATION: 6/99
PROJECT IDENTIFICATION: 962-23-08-33
NASA CONTRACT NO.: NAG8-115
RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Feigelson, R.S., De Mattei, R.C., and DeLucas, L. "Laser Scattering Tomography - a Technique for Studying Crystal Defects, Their Relationship to Growth Conditions and Their Effect on Diffraction." Protein Crystal Growth, Panama City Beach, Florida, April 29-30, 1996.

Role of Fluid Shear on 3-D Bone Tissue Culture

PRINCIPAL INVESTIGATOR: Prof. John A. Frangos

University of California, San Diego

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The ultimate goal of this research is the optimization of growth and differentiation of three-dimensional bone cell cultures *in vitro*. The research has medical implications in arresting bone loss due to microgravity, bedrest, and disuse, and in developing better implant devices and grafting materials. Our objective is to study the role of fluid shear stress on three-dimensional growth and differentiation of osteoblasts and to manipulate fluid shear stress throughout the culture period to maximize viable and differentiated tissue. Specifically, we will:

1. Determine the role of different levels of fluid shear stress on osteoblast growth differentiation when grown on porous collagen beads in a Slow Turning Lateral Vessel (STLV).
 - a. Study different levels of shear stress experienced by the cells in the bioreactor by using collagen beads that are either unweighted (minimal shear), weighted with small amounts of titanium particles (moderate shear), or weighted heavily with titanium particles (high shear) and compare them to similar beads in control situations (static in the incubator or immobilized in a trickle bed reactor system).
 - b. Evaluate the growth characteristics of the osteoblasts by determining growth rate and glucose consumption.
 - c. Perform cell cycle analysis by propidium iodine staining and flow cytometry on cells subjected to no, low, and high fluid shear stress. For completeness, we will also perform this analysis on monolayer cells exposed to well-defined levels of shear in our two-dimensional laminar flow system.
 - d. Assess differentiation by measuring alkaline phosphatase activity on the cell membrane, hydroxyapatite deposition onto the beads, and osteocalcin release into the media.
 - e. Assess cell organization and growth patterns on the porous beads by SEM analysis of bead samples.
 - f. Evaluate media PGE₂ levels for comparison to previous work on fluid shear stress on osteoblasts grown as monolayers on glass slides. This will serve as a comparison of two- and three-dimensional growth under flow and shear conditions.
2. Extend our knowledge of the role of fluid shear stress on cell differentiation to optimize the reactor conditions. In this part of the study, we will progress from constant shear level during the culturing period to variable shear levels throughout the culturing period in order to optimize growth and differentiation. These studies will include the following:
 - a. Determine if altering (increasing) the shear stress within a culturing period can promote differentiation.
 - b. Determine if reducing shear stress after the onset of differentiation results in the cells reverting to a proliferative phase.
 - c. Evaluate whether intermittent periods of increased shear stress are capable of providing the stimulus required for initiation.

Task Description:

Specific Aim 1: We propose to differentiate between the effects of no, low, and high fluid shear stress on osteoblasts in three-dimensional culture.

Specific Aim 2: We propose to optimize the reactor growth condition of osteoblasts on matrix beads by manipulating the hydrodynamics of the system. Altering the fluid hydrodynamics within a single culturing period will reveal the importance of fluid shear stress in bone tissue growth and differentiation. Changes in fluid shear stress within a culturing period may be achieved by altering the media density. The major force creating fluid shear stress on the beads is the force of gravity resulting in bead settling. The settling velocity is dependent on the density difference between bead and fluid. The greater the difference, the greater the settling velocity, thus the greater the fluid shear stress on the beads and cells. Thus, we propose that manipulation of media density, achieved with the normal medium changes, can alter the fluid shear in the system and promote osteoblast differentiation. Ficol 400 (Pharmacia) may be used to achieve altered densities. Ficol 400 is a neutral, highly branched, hydrophilic polymer of sucrose. It dissolves readily in aqueous solutions up to a concentration of 50% by weight and a specific gravity of 1.2 without exceeding normal osmolality. It is also cell culture tested by Sigma, but will be tested extensively on our osteoblast system before use. By utilizing media density to manipulate shear stress within the reactor, we will be able to alter the shear stress within a culturing period by approximately 3.5 dyne/cm^1 (i.e., from 0.5 to 4 or from 2 to 6 dyne/cm^2).

Task Significance:

In our lab, we have previously cultured primary rat osteoblasts and studied their response to fluid shear stress when grown as monolayers on glass slides (Reich et al., 1990; Reich and Frangos, 1991; 1993; Appendix) and when grown on macro-porous collagen beads in a fluidized bed bioreactor (VERAX System One) (Hillsley and Frangos, 1994; Appendix). The flow-induced shear stresses on the cells on the beads, assuming no bead tumbling and applying Stokes Law, were estimated to be on the order of dyne/cm^2 . The osteoblasts were evaluated for markers of differentiation, including alkaline phosphatase activity and hydroxyapatite formation. A control experiment was conducted in which osteoblasts were grown on the same macro-porous collagen beads under static conditions. Static beads had a better seeding efficiency, but the final cell density was similar to that of beads exposed to flow. The alkaline phosphatase (AP) levels per cell dropped earlier and more dramatically for the cells subjected to flow in the bioreactor than for the static cells. Studies by Owen et al., (1990) have shown that alkaline phosphatase mRNA levels peak just prior to the onset of mineralization. We observed a similar peak in alkaline phosphatase activity near the time that mineralization began. In comparable monolayer shear experiments, we also observed a drop in AP MRAN levels, followed by decreased AP activity (unpublished data). Hydroxyapatite greatly increased during the three-dimensional flow experiment. Yet in comparable static control studies, no measurable hydroxyapatite was detected in this time frame. This indicates that when coupled with three-dimensional growth, fluid flow promotes mineralization by osteoblasts *in vitro*. This type of cell culturing system shows great promise for growing a large number of osteoblasts.

The above described three-dimensional fluidized bed osteoblast culturing system produced differentiated cells. However, this system would be greatly improved if larger numbers of cells could be cultured prior to the onset of mineralization, and if a mixed cell population of differentiated and proliferating osteoblasts could be maintained throughout the culturing period. Both static and flow beads resulted in limited cell density due most probably to diffusion limitations in control beads and mechanical disruption of surface cells on reactor beads resulting from bead-bead and bead-reactor collisions. The STLTV offers an opportunity to increase the cell density prior to eliciting differentiation with increased shear stress.

The STLTV imposes shear based on settling velocities, a principle also utilized by the fluidized bed reactor. However, the STLTV configuration controls bead-to-wall bumping and turbulence better due to elimination of a need to recirculate media through a peristaltic pump. These are the main impediments to growth and differentiation (Cherry and Papoutsakis, 1988) within the fluidized bed system.

By studying the optimal culturing conditions of osteoblasts and bone tissue, we can gain an understanding of the requirements for healthy bone formation and of the missing elements of microgravity which result in reduced bone mass and possibly also in bone diseases such as osteoporosis. The results of this study will also aid in developing techniques for propagating autologous grafts and maximizing bone healing.

Progress During FY 1996:

In microgravity as well as in bed rest and osteoporosis of disuse, there is altered perfusion of bone by interstitial fluid. Decreases in interstitial fluid flow correlate with bone loss. The overall goal of this project is to establish the cellular basis and mechanism for this correlation. Specifically, here we will determine if increased fluid flow

through bone stimulates increased net formation of bone. We are using two models for this study. The first is an *in vivo* model, where interstitial fluid flow is increased by altering the venous pressure in the femur and tibia of the rat by venous occlusion. The occlusion, which is accomplished by a venous tourniquet or outright ligation, leads to increased bone marrow pressure and, therefore, increased cortical bone perfusion. An *in vitro* system is also being developed, where rat calvarial osteoblasts are grown on weighted three-dimensional matrices and are perfused by suspending in the STL.V.

Results from the *in vivo* rat models have supported the hypothesis. In particular, venous ligation and tourniquet both stimulated net bone mass. This was assessed by histomorphometry and gravimetric analysis. The increase in bone mass was attenuated by daily administration of the prostaglandin synthesis inhibitor indomethacin as well as the nitric oxide synthase inhibitor aminoguanidine. These studies are on-going.

The *in vitro* model is currently being established. In addition, osteoclast culture from marrow is also being developed. This will allow for co-culture of osteoblasts and osteoclasts.

Our results are consistent and supportive of the concept that interstitial fluid flow stimulates bone cells to produce increased mineral or inhibit bone resorption. Such studies will lead to clinical procedures and medical devices to prevent bone loss.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 8/95 EXPIRATION: 7/99

PROJECT IDENTIFICATION: 962-23-01-22

NASA CONTRACT NO.: NAG9-837

RESPONSIBLE CENTER: JSC

Microgravity Studies of Cell-Polymer Cartilage Implants

PRINCIPAL INVESTIGATOR: Lisa E. Freed, M.D., Ph.D.

Massachusetts Institute of Technology (MIT)

CO-INVESTIGATORS:

Langer, R.

Goodwin, T.J.

Vunjak-Novakovic, G.

Massachusetts Institute of Technology (MIT)

NASA Johnson Space Center (JSC)

Massachusetts Institute of Technology (MIT)

Task Objective:

The long-term objectives of our current studies are: (1) to assess the effects of *in vitro* culture conditions, microgravity in particular, on cartilage tissue morphogenesis, (2) to correlate the characteristics of engineered cartilage with bioreactor fluid dynamics in the form of physically and biologically sound mathematical models, and (3) to elucidate the mechanisms underlying the effects of microgravity on the structure and function of the engineered cartilage. Related practical objectives are to optimize bioreactor design and develop operating strategies for cultivating tissues under conditions of simulated and actual microgravity.

Task Description:

A simulated microgravity environment can be used to engineer cell-polymer tissue constructs, the size and shape of which are determined by a FDA approved, biocompatible, biodegradable scaffold with a defined three-dimensional (3D) shape and structure. In particular, fibrous polyglycolic acid (PGA) can be seeded with isolated cells (chondrocytes) and cultivated in rotating bioreactors to make cartilaginous tissue constructs for *in vitro* studies of tissue morphogenesis and/or *in vivo* implantation.

Task Significance:

Engineered cartilage (i.e., tissue constructs grown *in vitro* using isolated cells and biomaterial scaffolds) can be used *in vivo* to create subcutaneous neocartilage (in nude mice) and for joint resurfacing (in rabbits). Thus, it represents a biologically-based therapy for repairing cartilage damaged by congenital defects, arthritis, or trauma. We have shown that the structure of engineered cartilage depends on hydrodynamic forces during *in vitro* cultivation; this is similar to the known effects of environmental forces on tissue morphogenesis *in vivo*. For example, structural organization of bone and cartilage depends on the mechanical distribution of compressive and tensile stresses. Ground-based research utilizing rotating vessels (simulated microgravity) is expected to enhance our understanding of the principles governing tissue morphogenesis. Space studies (actual microgravity) can further extend the operating limits of these vessels. The same approaches and methodologies can also be applied to other cell-polymer model systems in order to engineer other clinically useful tissues.

Progress During FY 1996:

Specific Aim (1):

Establish methods to culture chondrocytes on 3D synthetic, biodegradable polymer scaffolds in a rotating vessel to regenerate cartilaginous tissue.

Constructs based on bovine calf chondrocytes and polyglycolic acid scaffolds were seeded in spinner flasks and transferred on day 3 to rotating vessels (110 mL STLVs). Within 3 months of cultivation in STLVs, tissue constructs were 8mm in diameter x 5mm thick and started to resemble natural bovine articular cartilage with respect to histological appearance, biochemical composition, and mechanical properties. Histologically, constructs consisted of uniformly distributed round cells within a compact cartilaginous extracellular matrix surrounded by a thin layer of flat cells and collagen. Quantitative image analysis showed that 3-month constructs and natural cartilage had comparable amounts of glycosaminoglycan (GAG). Biochemical analyses showed that 3-month constructs contained 8% more water, 10% less GAG, and 75% less total collagen per gram wet weight than natural cartilage. Mechanical testing of 1- and 3-month constructs gave preliminary values for static stiffness (0.11 - 0.15 kPa), dynamic stiffness (1.7 - 2.3 MPa at 30% strain, 0.1 Hz) and streaming potential (0.04 - 0.07 mV/% at 30% strain, 0.1 Hz).

Specific Aim (2): Assess bioreactor mixing under selected tissue culture conditions.

A perfused rotating vessel was designed that consisted of the annular space (120 mL) between two concentric cylinders with diameters of 5.75 cm and 2 cm. The vessel containing cartilage discs was simultaneously perfused with flow-visualization tracers and rotated such that the discs were maintained in a state of continuous free-fall. Convective mixing was generated by the settling discs, which oscillated, tumbled, formed wakes, and shed vortices. Fluid-dynamic parameters including construct settling velocity (2-3 cm/s), settling Reynolds number (114 - 207), Peclet number 3.8), and equivalent number of perfectly mixed vessels in series (1.1) demonstrated excellent mixing in conjunction with relatively low shear in rotating vessels under the operating conditions selected for the cultivation of tissue constructs.

Specific Aim (3):

Correlate the characteristics of engineered tissues with specific fluid dynamic parameters in order to optimize bioreactor operating conditions.

Bioreactor mixing conditions affected the structure and function of cell-polymer cartilage constructs as follows. Constructs grown from 1 month in STLVs had a significantly higher fraction and more uniform distribution of GAG than constructs grown for 1 month in spinner flasks. Histologically, constructs from STLVs were uniformly cartilaginous while constructs from flasks had outer capsules 0.3 mm thick consisting of multiple layers of flat cells and collagen but less than 5% of the total GAG. One-month constructs grown in STLVs had significantly better mechanical properties than 1-month constructs grown in spinner flasks.

Collaborations (MIT-JSC): A biotechnology flight study within the Shuttle-Mir program was launched on September 16, 1996 (STS-79) as described in our concurrent NASA grant titled "Microgravity Tissue Engineering."

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 3/94 EXPIRATION: 3/95

PROJECT IDENTIFICATION: 962-23-01-11

NASA CONTRACT NO.: NAG-9-65

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Bursac, P.M., Freed, L.E., Biron, R.J., and Vunjak-Novakovic, G. Mass transfer studies of tissue engineered cartilage. *Tissue Engineering*, 2, 141-150 (1996).

Freed, L.E. and Vunjak-Novakovic, G. Microgravity tissue engineering. *In Vitro Cell. Dev. Biol.*, (In Press).

Vunjak-Novakovic, G. and Freed, L.E. Cell-polymer system for tissue engineering. *Chemical Industry*, 49 (12), 511-519 (1996).

Vunjak-Novakovic, G., Freed, L.E., and Langer, R. Chondrocytes cultured on biodegradable polymers. *Synovial I. Rheumatologie*, 4-5 (April 1996).

Vunjak-Novakovic, G., Freed, L.E., Biron, R.J., and Langer, R. Effects of mixing on tissue engineered cartilage. *American Institute of Chemical Engineers Journal (AIChEJ)*, 42, 850-860 (1996).

Books/Chapters

Freed, L.E., Vunjak-Novakovic, G. "Tissue culture bioreactors: chondrogenesis as model system," in "Textbook of Tissue Engineering." Edited by: RP Lanza, R. Langer, W. Chick. R.G. Landes Company, Austin, Texas, Chapter 11, pp 150-158, 1996.

Presentations

Bursac, P., Vunjak-Novakovic, G., Biron, R., and Freed, L.E. "Mass Transfer Studies of Tissue Engineered Cartilage." Annual Meeting of the BMES, Boston MA, October 1995. 23: S-52.

Vunjak-Novakovic, G., Freed, L.E., and Langer, R. "Bioreactor Cultivation of Chondrocytes on Biodegradable Polymer Scaffolds." 5th World Congress of Chemical Engineering, San Diego, CA, July 1996.

Vunjak-Novakovic, G., Freed, L.E., and Langer, R. "Chondrocytes Cultured on Biodegradable Polymers." *Interventional Rheumatology: From Basic to Clinical Research*, Paris, France, March 1996.

Vunjak-Novakovic, G., Freed, L.E., and Langer, R. "Effects of Hydrodynamic Forces on Natural and Tissue Engineered Cartilage." Annual Meeting of the BMES, Boston, MA, October 1995. 23:S-59.

Microgravity Tissue Engineering

PRINCIPAL INVESTIGATOR: Lisa E. Freed, M.D., Ph.D.

Massachusetts Institute of Technology (MIT)

CO-INVESTIGATORS:

Vunjak-Novakovic, G.
Cohen, R.
Gooch, K.
Martin, I
Nerem, R.
Stamenovic, D.

Massachusetts Institute of Technology (MIT)
Massachusetts Institute of Technology (MIT)
Massachusetts Institute of Technology (MIT)
Massachusetts Institute of Technology (MIT)
Georgia Institute of Technology (GT)
Boston University (BU)

Task Objective:

Engineered tissues can be grown *in vitro* using isolated cells, three-dimensional (3-D) polymer scaffolds, and tissue culture bioreactors. Microgravity tissue engineering refers to the cultivation of cell-polymer tissue constructs in NASA rotating bioreactors in either: (a) unit gravity, by adjusting the vessel rotation speed such that the constructs are maintained in a state of continual free-fall ("simulated microgravity"), or (b) reduced gravity in space (actual microgravity). Our working hypothesis is that rotating bioreactors offer relatively well-defined fluid dynamic conditions that stimulate cells within constructs to maintain their differentiated phenotype and form-functional tissues. Freely suspended tissue constructs are grown in an environment that provides high supply rates of nutrients and gases while maintaining relatively low shear stresses. Long-term objectives of the project are to improve our basic understanding of tissue morphogenesis and to create functional tissues for a variety of clinical applications. The specific scientific and practical objectives are as follows:

- (1) Bioreactor studies of cartilage tissue morphogenesis: (MIT) (a) Study the effects of cultivation conditions and time on *in vitro* chondrogenesis. (b) Assess the effects of microgravity on cartilage tissue constructs in a five-month space study. (c) Evaluate bioreactor designs and operating strategies for further flight studies. (d) Optimize the cell-polymer-bioreactor system for microgravity tissue engineering.
- (2) Fluid-dynamic, mass transfer and metabolic studies: (GT) (a) Characterize the fluid-dynamic and mass transfer environments of tissue constructs in rotating vessels. (b) Study hydrodynamic effects on tumor cell spheroids. (c) Study the metabolic activities of cells in monolayers, spheroids and 3-D tissue constructs.
- (3) Structure-function relationships for cartilage tissue constructs: (MIT, BU) (a) Characterize construct structure with respect to the amounts and distributions of tissue components. (b) Study construct function (i.e., biomechanical behavior, matrix composition, synthesis and turnover rates). (c) Develop structure-function relationships for engineered cartilage in the form of mathematical models.
- (4) Extend the cell-polymer-bioreactor system for tissue engineering to a variety of cell types: (MIT) (a) cardiac, (b) bone, (c) endothelial, (d) mesenchymal.

Task Description:

A tissue engineering system based on isolated cells, 3-D synthetic, biodegradable polymer scaffolds, and tissue culture bioreactors will be used to study *in vitro* tissue morphogenesis with two long-term goals: 1) to make functional tissue implants for medical applications and 2) to optimize an *in vitro* system for tissue engineering. Cell-polymer cartilage constructs will be cultivated under a variety of hydrodynamic and physicochemical conditions, including simulated and actual microgravity, and assessed with respect to construct structure and function. A variety of studies are planned including correlating tissue morphogenesis with culture conditions and duration, quantitating flow, mass transfer and cell metabolism in bioreactors, developing structure-function relationships for engineered cartilage, and extending the same methodologies to studies of cardiac, bone, endothelial, and mesenchymal stem cell constructs. The project is realized through the joint efforts of research teams located at

the Massachusetts Institute of Technology (Specific Aims 1, 4, and part of 3), Georgia Institute of Technology (Specific Aim 2) and Boston University (part of Specific Aim 3), in cooperation with the NASA Johnson Space Center.

Specific Aim 1: Bioreactor studies of cartilage tissue morphogenesis. Cartilaginous tissue constructs will be grown using isolated chondrocytes, polymer scaffolds (e.g., 5-10 mm diameter disks, 2-5 mm thick, 97% porous) and tissue culture bioreactors (e.g., fed-batch and continuous flow rotating vessels, spinner flasks, and static vessels). The effects of bioreactor flow and mixing on cell seeding and the resulting constructs will be assessed. Tissue regeneration will be studied with respect to medium concentrations of nutrients, gases, growth factors and metabolites, and culture time. Bioreactor operating conditions will be designed to match the changing needs of the growing tissue over the course of *in vitro* cultivation. Correlations of tissue culture parameters with construct size, composition, morphology, and function will be developed and used to optimize the design of bioreactors for microgravity tissue engineering. A Shuttle-Mir flight experiment in which cartilaginous constructs will be grown for five months in an automated bioreactor system aboard the space station is scheduled to launch in September, 1996. Cell-polymer tissue constructs based on bovine chondrocytes will be prepared at 1g in simulated microgravity and transferred into the Biotechnology System (BTS). The BTS will travel via STS-79 to the Mir space station and operate in microgravity. A control experiment will be conducted on the ground in an otherwise identical BTS. At 1g, mixing will result from relative construct motion within the bioreactor vessel while in space, mixing will be achieved by differential rotation of the concentric cylinders that comprise the bioreactor vessel. Medium and gas exchange in the BTS will be provided by pre-programmed infusions and perfusions, respectively. System pH, gas, and glucose levels will be measured, and construct motion within the vessel will be videorecorded. Final tissue constructs will be analyzed with respect to cell viability, size, biochemical composition and histomorphology, and biomechanical properties.

Specific Aim 2: Flow, mass transfer and metabolic studies. Flow conditions and mass transfer in rotating bioreactors will be studied using a model bioreactor resembling the BTS with two concentric, independently rotated cylinders. Construct and fluid velocities will be measured using video tracking and particle-image velocimetry; concentration fields will be measured by recording the fluorescence of dye tracers for nutrients, gases, and metabolites. A theoretical model will be developed and used to infer the shear stress environment in the vicinity of the constructs and to quantitate mixing and mass transfer at the construct surface. A custom-made viscometer with uniform temporal and spatial shear stress distributions will be designed and used to study the formation and metabolic function of tumor cell spheroids. Correlations of spheroid structure and function with flow parameters will be developed and used to model cell-cell and cell-construct interactions in tissue engineering bioreactors. A custom-made perfusion system equipped for on-line NMR measurements will be used to study cell monolayers and 3-D tissue constructs over a range of cultivation conditions. Cell and tissue metabolism (e.g., oxygen and glucose consumption, matrix biosynthesis) will be studied as a function of flow conditions and concentrations of gases, nutrients, and metabolites.

Specific Aim 3: Structure-function relationships for cartilage tissue constructs. Construct composition and morphology will be quantitated over the course of *in vitro* cultivation using a combination of biochemical, histological, mass transfer, image processing and NMR techniques. Biosynthesis rates of matrix components will be measured (e.g., with radioactive tracers) and used in conjunction with various tissue-typing methods (e.g., quantification of collagen types I & II, labeling of enzymes and metabolites) to assess cellular activity within constructs.

Construct and cartilage biomechanics will be tested in confined and unconfined compression and in shear to independently determine elastic parameters (i.e., Young modulus, aggregate modulus, Poisson's ratio, shear modulus). These will be used in conjunction with a biphasic theory to estimate other parameters (e.g., hydraulic permeability, deformation time constants) needed to explain and predict the mechanical behaviors of the tissues under different loading regimes (e.g., stress-relaxation, oscillatory loading). Microstructural models will be developed from mechanical, biochemical and histological data and used to assess relative contributions of glycosaminoglycan (GAG) and collagen to the mechanical behavior of the tissues. These models will form a framework to study structure-function relationships in natural and engineered cartilage.

Specific Aim 4: Extend the cell-polymer-bioreactor system for tissue engineering to a variety of cell types. The model system developed for cartilage tissue engineering (i.e., rotating bioreactor cultivation of chondrocytes on 3-D biodegradable polymer scaffolds) will be extended to other cell types including cardiac, bone, endothelial, and mesenchymal stem cells. *In vitro* cultivation conditions will be optimized over a wide range of cellular metabolic rates and shear tolerances. In particular, each cell type will be studied using various polymer scaffolds (e.g.,

dimensions, 3-D structure), bioreactors (e.g., lower shear rotating vessel vs. higher shear spinner flask), and culture conditions (rates of nutrient supply, gas exchange and waste removal). Cardiac cells will be used to regenerate contractile tissue constructs for studies of the effects of hypoxia, drugs and simulated microgravity on cardiac tissue function. Physiological studies will be carried out by recording and mapping cardiac potentials in unpaced and paced tissue constructs. Osteoblasts will be used to form tissue-engineered bone for potential use in orthopaedic surgery. Studies will be done to select an optimal cell source and scaffold (e.g., structure and biodegradation rate) and to determine culture conditions associated with matrix calcification. Endothelial cells will be used to explore the *in vitro* formation of capillary networks to pre-vascularize tissue engineered constructs. Mesenchymal stem cells (i.e., bone marrow derived stromal cells) will be cultured in the presence of growth factors, hormones, and metabolites to study *in vitro* cell differentiation (i.e., osteo- and chondrogenesis).

Task Significance:

Basic research in the area of microgravity tissue engineering has broad practical and scientific significance. *In vitro*-grown 3-D tissue constructs that structurally and functionally resemble natural tissues would represent ideal substitutes for lost or damaged tissues. Key tissue engineering requirements include: 1) a 3-D scaffold for cell attachment and 2) a bioreactor to maintain physicochemical and hydrodynamic parameters within optimal ranges for tissue morphogenesis. We previously demonstrated the feasibility and advantages of using a cell-polymer-bioreactor system for engineering cartilage and more recently extended this work to several other cell types (i.e., cardiac, bone, endothelial, and mesenchymal).

Cultivation of cell-polymer tissue constructs under conditions of simulated microgravity (rotating vessels at 1g) appears to enhance cartilage tissue formation. The effects of actual microgravity, however, can only be studied in space. Data are already available from pilot space studies, including a demonstration of cell growth and metabolic function in chondrocyte monolayer cultures aboard STS-62 (2/94). Our ongoing work in the area of microgravity tissue engineering and related experiments planned within the Shuttle-Mir program provide a unique opportunity to determine the effects of gravitational forces on cartilage tissue constructs in parallel ground and space studies.

The current project was designed to integrate research in several areas critical for advancing our basic understanding of tissue morphogenesis and the *in vitro* cultivation of engineered tissues for medical use (i.e., tissue repair). Scientific studies conducted using the cell-polymer-bioreactor system will enable us to control and thereby study the effects of specific tissue culture parameters on cell growth and function. Bioreactor optimization is expected to lead to long-term cultivations of a variety of cell-polymer tissue constructs for both ground and space studies.

Progress During FY 1996:

Specific Aim (1):

(a) Bioreactor studies of cartilage tissue morphogenesis (Massachusetts Institute of Technology)

Cell-polymer cartilage constructs (5-10mm diameter, 3-6mm thick) were cultured for up to 3 months under various mixing conditions (rotating vessels, mixed spinner flasks, static flasks, mixed and static Petri dishes). Cell seeding was best achieved in spinner flasks in which >95% of the cells uniformly attached throughout the porous polymer scaffold over 12-18 hours. Mixing during subsequent tissue cultivation significantly improved the size, biochemical composition, and histomorphology of the resulting tissue constructs. *In vitro* cultivation of explants of natural cartilage under the above mixing conditions demonstrated essentially the same effects observed for engineered cartilage. On going studies include quantitating rates of synthesis and release of matrix components and evaluating the roles of growth factors, shear-protective agents, and nitric oxide on chondrogenesis. For example, adding IGF-I to the culture medium significantly increased construct size and glycosaminoglycan (GAG) content.

Cell-polymer cartilage constructs were cultured in rotating vessels, and the conditions of medium and gas exchange were systematically varied. Cell metabolism (i.e., rates of glucose utilization and the production of lactate, ammonia, and GAG) was assessed and correlated with culture conditions. Target set-ranges for cultivation parameters were established based on biochemical compositions and histomorphologies of the resulting tissue constructs. In particular, cultivation in rotating vessels (110 mL STLVs) for up to 3 months at pH = 6.9 - 7.25, pCO₂ = 40 - 80 mm Hg, and pO₂ = 80 - 120 mm Hg resulted in constructs that were histologically cartilaginous and contained cells (>90% viable), GAG (90% as much as natural cartilage per gram wet weight) and collagen (25% as much as natural cartilage per gram wet weight).

(b) Shuttle-Mir flight experiment (Massachusetts Institute of Technology, Johnson Space Center)

A total of six developmental ground studies (#1-6) were completed and a Shuttle-Mir flight study was started using cell-polymer constructs cultured first in simulated microgravity at MIT and then in the Biotechnology System (BTS) at JSC. Ground studies were designed to match the constraints of the actual space study, i.e., limited amounts of feed medium (10 L in 0.8 L aliquots) and gas for medium oxygenation and pH control (780 L). It was determined that the contents of the feed bag, which was held at 37°C, should be replaced at 10-14 day intervals to prevent degradation of medium components. The BTS system provided good control of medium pO_2 , pCO_2 , pH and glucose for metabolically active tissue constructs under the following operating conditions: (a) slow, continuous glow of gas from a premixed tank into the gas exchanger (e.g. 10% CO_2 /90% air at 0.6 mL/min), and (b) intermittent perfusion of medium through the gas exchanges such that the volume recirculated at each perfusion was comparable to that of the bioreactor vessel.

The length of the BTS cultivation ranged from several days in studies 1-2 to four months in study 4; studies 5 and 6 verified actual flight hardware performance for 5 weeks. In studies 1 through 3, constructs were not metabolically active (this was associated with high system pH), and had low final weights and GAG contents. In studies 4 through 6, constructs were metabolically active and culture parameters were maintained within target ranges (pH - 7.0 - 7.45, pCO_2 = 40 - 75 mm Hg, pO_2 = 80 - 100 mm Hg and glucose = 2.5 - 4.0 g/L). Constructs from study 4 had significant amounts of GAG while constructs from studies 5 and 6 had very high amounts of GAG and cartilaginous histomorphologies. Cells isolated from the four-month constructs were 95% viable.

Data obtained from ground studies 1 through 6 were used to specify operating conditions for the flight study: gas exchange by perfusion of 4 mL/min for 20 minutes four times per day and medium exchange by infusion of 60 mL per day. Sixty constructs were cultivated in simulated microgravity starting at MIT on 6/19 for 3 months (including the 6 week launch delay). Ten constructs each were transferred into two identical BTSs at KSC on 9/12. One BTS was launched on 9/16 via STS-79 to the Mir space station; the other was transferred to JSC to serve as a ground control. Medium samples from both units on 10/2 and 10/8 indicated that culture parameters were within target ranges (pH = 7.18 - 7.36, pCO_2 = 44 - 60 mm Hg, pO_2 = 109 - 127 mm Hg and estimated glucose = 3.6 - 3.8 g/L). The flight study, currently on day 30, already represents the longest cell cultivation conducted in microgravity.

Specific Aim (2): Fluid-dynamic, mass transfer and metabolic studies (Georgia Institute of Technology)

A prototype rotating vessel resembling the bioreactor in the BTS was designed for investigating the motion of constructs and fluid flow fields in their vicinities using the technique of particle image velocimetry. The vessel consists of a pair of concentric cylinders that are mounted horizontally with respect to gravity and are capable of independent rotation. Several methods were analyzed for providing a uniform sheet illumination of a portion of the flow field around the construct (i.e., using liquid with a refractive index matching that of the outer cylinder).

A concentric-cylinder viscometer with uniform temporal and spatial shear stress distributions was designed to study tumor cell spheroids in a well-controlled and quantifiable hydrodynamic environment. A large shearing volume allows sampling over long periods of time under constant hydrodynamic conditions. Related protocols were designed for culturing the tumor cell spheroids in a range of flow regimes.

Methods were developed to measure cell metabolism and extracellular matrix production in monolayer cultures of bovine chondrocytes cultured in 5% CO_2 incubators. The ratio of lactate to glucose was 1.0 - 1.1 mol/mol indicating that the cells were well oxygenated. The release of soluble GAG was highest after one week in culture (0.2 μ g/hr per 10^6 cells), after which it decreased and stabilized at a ten-fold lower level. A continuous sheet of extracellular matrix formed over six weeks of culture. The design of a perfusion system for quantitating oxygen consumption and the metabolic rates of chondrocytes at various levels of dissolved oxygen and pH is currently in progress.

Specific Aim (3): Structure-function relationship for cartilage tissue constructs (Boston University, Massachusetts Institute of Technology)

The structure and function of cartilage constructs grown in rotating bioreactor vessels have been assessed with respect to morphology (quantitative histology) biochemical composition (amounts of tissue components), mass

transfer properties (diffusion studies), and biomechanical properties (compression studies). The amount and spatial uniformity of cartilaginous matrix and the stiffness of constructs all increased and the permeability decreased with cultivation time. Further development of the above correlations are currently in progress.

Explants of bovine articular cartilage were studied using confined and unconfined creep tests in a series of loading steps. A transversely isotropic biphasic model is being used to estimate Young moduli, Poisson's ratios, and permeabilities in axial and radial directions. Young moduli and permeabilities were within the range of values previously reported in the literature but showed dependencies on the applied stress while Poisson's ratios decreased with increasing applied stress.

In contrast, when the same model was applied to data obtained for tissue-engineered cartilage in a single step creep test, Poisson's ratios were virtually independent of the applied stress. This suggests that natural and engineered cartilage resist deformation via different mechanisms and that Poisson's ratios can indicate such a difference. Independent measurements of Poisson's ratios using stress transducers on radially confined samples are currently underway to verify the predicted differences in the Poisson's ratios behavior of normal and engineered cartilage. The model is currently being tested using data obtained from independent stress-relaxation tests.

A two-dimensional microstructural model of collagen matrix viewed as a network of interconnected hexagons and glycosaminoglycan (GAG) as a pressurized elastic fluid is currently under development. The model is being used in conjunction with measured biomechanical properties to study the respective contributions of GAG and collagen to construct biomechanics.

Specific Aim (4): Extend the cell-polymer-bioreactor system for tissue engineering to a variety of cell types. (Massachusetts Institute of Technology)

Cardiac cells isolated from 9 to 5 day-old chick embryos were seeded on polymer scaffolds (10 mm diameter, 2 mm thick) and cultivated for up to four weeks in rotating vessels and spinner flasks. Cardiac tissue constructs were evaluated electrophysiologically and histologically. Constructs grown in pilot studies contracted spontaneously and synchronously; histology indicated some features of striated muscle. A system for high-resolution mapping of cardiac potentials consisting of 36 microelectrodes has been fabricated for *in vitro* physiological and pharmacological studies. Biochemical methods to detect specific cardiac tissue markers (e.g., creatine phosphokinase, myosin) are under development.

Passaged rat calvarial osteoblasts were seeded on polymer scaffolds with or without a polylactic acid coating and cultured for up to four weeks in rotating vessels and spinner flasks. Histological assessment showed cells and initial calcification of the tissue matrix. Biochemical methods to detect specific bone tissue markers (e.g., alkaline phosphatase, osteocalcin, collagen types I and III) are under development.

Bovine aorta endothelial cells were seeded on polymer scaffolds and cultured for one week in spinner flasks. Histological assessment showed cell monolayers on scaffold fibers and the formation of capillary tubes between fibers. Methods to detect endothelial cell markers (e.g., factor VIII) are under development.

Mesenchymal stem cells (i.e., bone marrow derived stromal cells from chick embryos and bovine calves) were expanded in monolayers, seeded on polymer scaffolds, and cultured for up to four weeks in spinner flasks in the presence of various differentiation factors. Certain conditions (β -FGF, IGF-I, TGF- β , dexamethasone) promoted cartilage development (i.e. constructs contained GAG) while other conditions (β -glycerophosphate, dexamethasone) promoted bone development (i.e., constructs contained foci of mineralized matrix).

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 9

TASK INITIATION: 9/95 **EXPIRATION:** 8/99

PROJECT IDENTIFICATION: 962-23-01-11

NASA CONTRACT NO.: NAG9-836

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Bursac, P.M., Freed, L.E., Biron, R.J., and Vunjak-Novakovic, G. Mass transfer studies of tissue engineered cartilage. *Tissue Engineering*, 2:141-150 (1996).

Freed, L.E. and Vunjak-Novakovic, G. Microgravity tissue engineering. *In Vitro Cell. Dev. Biol.*, (In Press).

Vunjak-Novakovic, G. and Freed, L. Cell-polymer system for tissue engineering. *Chemical Industry*, 49, (12)511-519 (1996).

Vunjak-Novakovic, G., Freed, L.E., and Langer, R. Chondrocytes cultured on biodegradable polymers. *Synovial J. Rheumatologie*, 4-5 (April 1996).

Vunjak-Novakovic, G., Freed, L.E., Biron, R.J., and Langer, R. Effects of mixing on tissue engineered cartilage. *American Institute of Chemical Engineers Journal (AIChEJ)*, 42:850-860 (1996).

Books

Freed, L.E. and Vunjak-Novakovic, G. "Tissue Culture Bioreactors: Chondrogenesis as a Model System," in "Textbook of Tissue Engineering." Edited by: RP Lanza, R, Langer, W. Chick. R.G. Landes Company, Austin, Texas, Chapter 11, pp 150-158, 1996.

Presentations

Bursac, P., Vunjak-Novakovic, G., Biron, R., and Freed, L.E. "Mass Transfer Studies of Tissue Engineered Cartilage." Annual meeting of the BMES, Boston MA. October ,1995, 23:S-52.

Gooch, K.J., Langer, R., Freed, L.E., and Vunjak, G. "In Vitro Vasculogenesis." Annual Meeting of the BMES. University Park, PA. October, 1996.

Obitz, T.W. "Mechanical properties of articular cartilage and tissue engineered constructs: a transversely isotropic analysis." S.M Thesis, Boston University, Boston, MA, Vunjak-Novakovic G on Thesis Committee, Stamenovic D, Advisor, September, 1996.

Obitz, T.W., Eisenbery, S.R., and Stamenovic, D. "Creep Behavior of Calf Articular Cartilage: a Transversely Isotropic Analysis." Annual Meeting of the BMES, University Park, PA. October , 1996.

Vunjak-Novakovic, G., Freed, L.E., and Langer, R. "Bioreactor Cultivation of Chondrocytes on Biodegradable Polymer Scaffolds." 5th World Congress of Chemical Engineering, San Diego, CA. July, 1996.

Vunjak-Novakovic, G., Freed, L.E., and Langer, R. "Chondrocytes Cultured on Biodegradable Polymers." *Interventional Rheumatology: From Basic to Clinical Research*, Paris, France. March, 1996.

Vunjak-Novakovic, G., Freed, L.E., and Langer, R. "Effects of Hydrodynamic Forces on Natural and Tissue Engineered Cartilage." Annual Meeting of the BMES, Boston, MA. October 1995. 23:S-59.

Protein and DNA Crystal Lattice Engineering

PRINCIPAL INVESTIGATOR: Dr. D. T. Gallagher

Center for Advanced Research in Biotechnology

CO-INVESTIGATORS:

Gilliland, G.L.

Center for Advanced Research in Biotechnology (CARB)

Task Objective:

- 1) To enhance scientific understanding of the molecular interactions that control crystal growth.
- 2) To produce crystal contact mutants of the enzyme subtilisin and compare their crystal growth to that of wild-type.
- 3) To produce branched-DNA oligomers and study their structure using crystallography and other methods.

Task Description:

Standard molecular biology techniques will be used to make site-specific mutants of the enzyme subtilisin BPN', which will then be crystallized using acetone. DNA that has been designed to contain stable branched structures will be synthesized and characterized by electrophoresis, UV spectroscopy, and other methods. Crystallization of the DNA will be studied, and crystals analyzed by diffraction.

Task Significance:

Current advances in medical and other biotechnologies depend on knowing the precise structures of molecules as determined through crystallography. To do this you need crystals, but how protein and DNA crystals grow is still largely a mystery. These studies are aimed at the fundamental mechanisms of crystal growth. The balance of forces that operate in one well-characterized protein crystal system (primitive monoclinic subtilisin) will be measured by modifying key residues in the crystal contacts. In addition, the structure of branched DNA, which is important in many biological processes as well as potential synthetic biomaterials, will be investigated.

Progress During FY 1996:

During FY96, the first full year of the project, the following advances were made. In the protein part of the project, a paper laying the groundwork for future subtilisin crystal growth studies has been accepted by Acta Cryst., and crystal growth studies on several mutants are underway. A new protein with several crystal forms, threonine deaminase, has been analyzed by diffraction and the growth of 3 polymorphs compared. In the DNA subproject, a compound junction with tetrahedral topology has been designed and its components synthesized, purified and assembled, a step toward lattice construction. Two designs for rigid DNA duplex triangles have been developed and the components have been synthesized and purified, and a more ambitious DNA assembly, a rigidized Holliday junction, has been designed.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-23-08-37

NASA CONTRACT No.: H-25793D

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Gallagher, T., Oliver, J., Bott, R., Betzel, C., and Gilliland, G.L. The structure of subtilisin BPN' at 1.6A resolution and three high-resolution crystal forms compared. Acta Crystallographica D., (accepted for publication 5/96).

Microgravity-Based Three-Dimensional Transgenic Cell Models

PRINCIPAL INVESTIGATOR: Steve R. Gonda, Ph.D.

NASA Johnson Space Center (JSC)

CO-INVESTIGATORS:

Yang, T.C.

Wu, H.

Richmond, R.C.

Provost, S.

Fritz, P.

NASA Johnson Space Center (JSC)

KRUG Life Sciences

Dartmouth College

Stratagene, Inc.

USRA

Task Objective:

The FY '96 objective is to continue the development of three-dimensional cell culture models that have been genetically engineered to contain multiple copies of a defined target gene for mutational analysis.

Task Description:

Cell culture experiments will be conducted in the NASA-designed bioreactors to find optimal conditions for growing stable, three-dimensional, tissue-equivalent assemblies. Rat and human fibroblast and epithelial cells will be co-transfected with Stratagene's Big Blue 45.5 Kb Shuttle vector lambda bacteriophage DNA containing the lambda/lac I shuttle vector and the plasmid psv2NEO. Culture of fibroblasts in various combinations with epithelial cells and microcarrier systems will be evaluated and optimized with primary focus on (i) cell attachment, (ii) cell growth and proliferation, and (iii) stability of three-dimensional structures. After seeding bioreactors with cells and microcarriers, cell attachment and proliferation, three-dimensional formation and stability, extracellular matrix composition and organization, and general morphology of the three-dimensional models will be evaluated.

Task Significance:

Advances on two fronts of biotechnology are merged to provide new and fundamental information on the roles of multicellular organization in genetic alterations caused by exposure to environmental conditions. Advances in genetic engineering of cells and advances in the development of three-dimensional models in the NASA bioreactor that are representative of multicellular tissue will be utilized to develop three-dimensional functional models for risk assessment of environmental insults.

Progress During FY 1996:

Considerable progress was made last year toward developing and optimizing three-dimensional cell culture models that have been genetically engineered to contain a defined target gene for mutational analysis. In the service of this project goal, we conducted experiments to find optimal conditions for growing three-dimensional, tissue-equivalent cell culture models in the NASA-designed bioreactors, High Aspect Ratio Vessel (HARV) and the Slow Turning Lateral Vessel (STLV) (both manufactured by Synthecon, Inc.). Cultures of selected fibroblasts in various combinations with epithelial cells and microcarrier systems, were evaluated in these vessels with the primary focus on (i) cell attachment, (ii) cell growth and proliferation, and (iii) the stability of three-dimensional structures. Spheroids formed on bioresorbable scaffolds by the attachment, growth, and proliferation of transgenic fibroblasts, and epithelial cells in coculture showed suitability as a stable three-dimensional model.

We used both human and rat epithelial cells and cell lines, cultured alone and in combination with Stratagene's Big Blue™ rat cell line, Rat 2 lambda. This cell line was derived from Rat 2 embryonic fibroblast cells (ATCC CRL 1764) that had been transfected with the pSV2NEO plasmid and cotransfected with Stratagene's Big Blue™ 45.5 kb shuttle vector. This cell line contains multiple copies of the lac repressor target gene. The vector is integrated separately into two of the Rat 2 mid-size chromosomes and as such serves as a sensitive molecular tool to score mutational effects of environmental insults.

Other cell types selected for culture included rat intestine epithelial IEC-6 (ATCC CRL 1592), human mammary epithelial (H184B5F5M10 growth variant) and human foreskin fibroblast (AGO 1522B). Immortal cell lines were tested for transformation using standard assay. All transfected cells were checked for karyotype before and after transfection.

After bioreactors were seeded with cells and microcarriers, they were monitored daily for cell number and viability, glucose utilization, pH changes, dissolved gases (pO_2 , pCO_2) and bicarbonate. Cell attachment, growth, and aggregate formation was monitored by phase contrast microscopy and documented with image capture microscopy. Cell samples were taken periodically, fixed in Omnifix™, and paraffin-embedded for histological analysis.

All cells grown as mono- and co-cultures in the bioreactors could attach and form aggregates, whether cultured with or without polyglycolic and polylactic bioresorbable scaffolds. In general, a greater percentage of viable fibroblasts (80% attached within the first 24 hours than did epithelial cells (50%); at 48 hours 93% of fibroblasts and 60% of epithelial cells had attached. The viability of unattached cells dropped to 1% by the third day of culture.

The growth and proliferation of attached cells varied greatly depending on cell type. Epithelial cells generally showed poor growth and proliferation in monocultures, with or without microcarriers. On the other hand, fibroblasts under the same conditions grew and proliferated well and expanded readily throughout the scaffolds. Cultured together, fibroblasts and epithelial cells continued to grow and proliferate over the entire 15-day culture period, forming three-dimensional assemblies.

Although three-dimensional aggregates were formed in all of the culture combinations used, differences were observed in aggregate size and stability, and in cellular and extracellular organization. Aggregates formed by epithelial cells in monoculture began to degrade by day 4, whereas aggregates formed by fibroblasts under the same conditions remained stable throughout 10-day experiment periods.

Spheroids formed from cocultures of epithelial cells and transgenic fibroblasts were stable throughout the 15-day culture period. Preliminary results indicate that both epithelial cells and fibroblasts are involved in the formation of cellular arrays within the core and along the surfaces of the aggregates. Amounts and organization of an extracellular matrix that formed within spheroids are being examined and characterized. The presence of apoptotic bodies, necrotic cells, and cell debris in spheroids indicates that further optimization of the cell culture model is needed.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/95 EXPIRATION: 8/99
PROJECT IDENTIFICATION: 962-23-01-30
RESPONSIBLE CENTER: JSC

Lymphocyte Invasion Into Tumor Models Emulated Under Microgravity Conditions In Vitro

PRINCIPAL INVESTIGATOR: Mr. Thomas J. Goodwin, M.S.

NASA Johnson Space Center (JSC)

CO-INVESTIGATORS:

Pellis, N.R.

Wolf, D.A.

Becker, J.

NASA Johnson Space Center (JSC)

NASA Johnson Space Center (JSC)

University of South Florida

Task Objective:

This application tests the hypothesis that microgravity provides a unique environment to create three-dimensional tumor models for the investigation of solid tumor invasion by human lymphocytes in vitro. We predict that this research will demonstrate that human lymphocytes oriented proximally to solid tumor models will be induced to invade and kill modeled tumor tissue. Two solid tumor models will be adopted from the NASA Rotating-Wall Vessel (RWV) bioreactor to propagate materials currently investigated by the applicant laboratory. Colon and breast cancer tissues co-cultivated with mesenchymal components yield tissue masses consistent with the investigation of the lymphatic invasion of human solid tumors. Tissue masses will be co-cultivated in stationary phase and RWVs with human peripheral blood lymphocytes (PBL) and with IL-2-activated PBL known as lymphokine activated killer (LAK) cells. Invasiveness will be analyzed quantitatively for adherence to lymphocyte populations to target tumors masses, the extent of infiltration, and the effect on tumor viability.

Previous investigations have shown that lymphocyte movement in simulated and true microgravity is substantially impaired when measured in type I collagen. The tumor models will be analyzed under the same conditions to determine if lymphocyte movement in native tissue rather than gelled collagen is profoundly affected by alterations in gravity load and vector.

The investigations will be the RWV technology in two applications: 1) production of tissue organoids and 2) analysis of the effect of gravity on lymphocyte movement. Completion of this proposed investigation will provide the experimental basis for establishment of three-dimensional models to investigate therapeutic strategies whether immunological, chemical, or radiological. Furthermore, it will facilitate identification of the utility of microgravity in two areas of cell biology: tissue production and cellular movement.

Finally, in the later stages of experimentation, solid tumors created in simulated microgravity will be transitioned into true microgravity in a Space Shuttle experiment where they will be inoculated with LAK cells, and the progress of these lymphocytes, activated and non-activated, will be measured via histological, immunohistochemical, and biochemical techniques.

Task Description:

Hypothesis:

Microgravity provides a unique environment to create three-dimensional tumor models for the investigation of the solid tumor invasion by human lymphocytes in vitro.

Specific Aim 1: Develop the models of choice: a) colon tumor model and b) breast tumor model.

Specific Aim 2: Quantitate the degree of invasion into the tumor models by resting and activated normal PBL: a) Analyze adherence of lymphocytes to tumor models and b) Immunohistochemical evaluation of invasion by location and distance traveled.

Specific Aim 3: Determine if lymphocyte invasion into tissue involves a normal locomotory response: a) test invasion in the RWV known to inhibit PBL locomotion into solid matrix, b) determine if lymphocyte activation in situ facilitates invasion in unit and microgravity, and c) determine the relationship of cytokines produced by tumors to invasion.

II. MSAD Program Tasks — Ground-based Research

Specific Aim 4: Determine the effect of tumor invasion by lymphocytes on cell metabolism and death: a) determine changes in cellular metabolic activity as a result of LAK invasion in tumors, b) analyze cell death in LAK infiltrated tumors, and c) distinguish if cell death is necrotic or apoptotic.

Specific Aim 5: Determine the effect of true microgravity on invasive process by LAK cells.

Task Significance:

It is of paramount importance to understand the response of the immune system to tumors. In many cancers, the host immune system is triggered, deployed systematically, and even has its cells accumulate at the site of the tumor. Despite what appears to be an overwhelming hemostatic response to destroy the tumor, the immune system seems to lose effectiveness at the tumor site. Therefore, it is critical that we model the tumor site to address strategies that will augment host immunity in cancer. Colorectal and breast carcinoma are the second and third largest cancer killers in the United States with 57,000 deaths occurring from colon and 46,000 deaths occurring from breast carcinoma in 1993. An estimated 153,000 new cases of colorectal carcinoma will occur along with an estimated 183,000 new cases of breast carcinoma. These carcinomas kill through either local or distant spread when the tumors metastasize. Survival of patients afflicted with colonic and breast carcinoma has not improved dramatically in recent decades, and the mechanisms for control of the metastatic process are poorly understood. Over the last four years, the NASA Johnson Space Center has developed in vitro tumor models using RWVs in several cell systems. Colon, breast, ovarian, and prostate cancer are but a few. Construction of these three-dimensional, in vitro tumor models has revealed striking similarities to tissues grown in vivo. In addition to the solid tumor models that have been created for study of the respective diseases, normal cellular models have also been created to study cell/cell interactions and the development of interstitial and cellular matrices which form in vivo. Recently, space flight experiments conducted in actual microgravity aboard the Space Shuttle have revealed characteristics of locomotion through solid matrix by normal human PBL. The mechanisms involved in the locomotion of PBL initiated in microgravity is currently under study; however, ongoing investigations have elucidated methodologies to elicit locomotion from PBL under normally non-locomotory conditions which rule out the necessity for chemical inducement. These methodologies may be employed to arrest solid tumors prior to metastasis by activation of lymphocytes at the tumor site. Three-dimensional tumor models developed in microgravity allow the study of this scenario.

Progress During FY 1996:

Substantial progress has been made in establishing that randomized gravity (simulated microgravity [SM]) provides a unique environment of low shear and turbulence to create three-dimensional (3D) tumor tissue models. Solid tumor models of colon (LS174T) and breast (MCF-7) cancers were established in rotating-wall vessel (RWV) culture to study the induction of lymphokine-activated killer (LAK) cells that invade and kill solid tumors. LS174T and MCF-7 were grown in RWV and stationary culture for 21 days on cultispher-GL microcarriers (Hyclone Labs) and GTSF-2 medium (Goodwin, *et al.*, 1993). Cells were seeded at 2.0×10^5 cells/ml with 1 mg/ml microcarriers. Stationary LS174T and MCF-7 cultures achieved average densities of 9.6×10^5 and 1.07×10^6 , while RWV cultures achieved 1.92×10^5 and 8.3×10^6 cells/ml. Glucose utilization rates at 21 days of culture for LS174T ranged from 4.2 and 1.27 mg/dl/hr in stationary phase to 6.4 and 2.98 mg/dl/hr in RWV culture, respectively. LS174T RWV cultures were positioned for known differentiation markers such as sucrase-isomaltase, villin, and desmin and expressed an increase in normal colon antigen a(NCA). Similarly, MCF-7 RWV culture displayed Estrogen receptor (ER⁺) Keratin 8,18,19 and polymorphic epithelial mucin-positive cells. LS174T and MCF models both expressed apical polarized, microvillus surfaces.

Specific Aim #1 - Develop the models of choice: a) tumor models and b) breast tumor models. Elements of Specific Aim #1 have been achieved as evidenced by the publication and presentation to the Society for In Vitro Biology in June, 1996.

Specific Aim #4 - Determine the effect of tumor invasion by lymphocytes on cell metabolism and death: a) Determine changes in cellular metabolic activity as a result of LAK invasion in tumors, b) Analyze cell death in LAK-infiltrated tumors, and c) Distinguish if cell death is necrotic or apoptotic. Elements of Specific Aim #4 have been partially achieved. Element a is being studied and quantitated at this time in both the breast and colon carcinoma model. Element b is also being studied at the present time, and one of the next steps will be to distinguish if cell death is either necrotic or apoptotic in nature. This will be determined by chromium release assay, which is to be performed on both models

after inoculation with LAK cells within the next six months.

Thus, the development of differentiated 3-D tissue assemblies in SM of colon and breast provide the plausible models to investigate the process of LAK cell adherence and invasion into solid tumor *in vitro*.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 8/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-23-01-32

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Goodwin, T.J., Canales, D.D., and Baker, T.L. "Three-dimensional tumor modeling for use in lymphokine-activated killer cell invasion.." 1996 world Congress on In Vitro biology, San Francisco, California, June 22-27, 1996.

Differentiation of Cultured Normal Human Renal Epithelial Cells in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Timothy G. Hammond

Tulane University

CO-INVESTIGATORS:

Lelkes, P.I.

Goodwin, T.J.

Albrecht, R.M.

Univ. of Wisconsin - Milwaukee Clinical Science Center

NASA Johnson Space Center (JSC)

University of Wisconsin, Madison

Task Objective:

Renal tubular injury is a common, lethal problem costing many billions of federal health care dollars annually. Although the molecules postulated to mediate many forms of this injury have been identified in vivo (The "Heymann antigen"/megalin (gp330) and an intermicrovillar glycoprotein (gp280)), the field is impeded by the lack of culture conditions in which kidney epithelial cells contain to express these highly differentiated nephrotoxin receptors; recent evidence suggests that gp330 is the polybasic aminoglycoside receptor. The purpose of this proposal is to explore microgravity as an innovative modality of cell culture which will lead to organ-specific differentiation of normal human renal epithelial cells expressing gp280 and gp330 in vitro.

Normal human renal cells have been difficult to obtain, cumbersome to purify, and impossible to maintain in differentiated form in culture. Our hypothesis is that simulated microgravity culture will provide a source of differentiated normal human epithelial cells expressing gp330 and gp280 in culture.

Task Description:

The specific objectives of this proposal are:

1. To compare enhancement of adhesion, proliferation, and organ-specific differentiation of renal epithelial cells in simulated microgravity (NASA rotating-wall perfused vessels) to conventional cell culture techniques (2-D monolayer, suspension culture, beads, polarization on Milipore inserts).
2. To test whether organ specific co-culture with cortical microvascular endothelial cells enhances adhesion, proliferation, and organ specific differentiation of renal epithelial cells in simulated microgravity (NASA rotating-wall perfused vessels) and conventional cell culture techniques.

Indices of organ-specific epithelial cell differentiation include expression of the postulated injury mediators gp280 and gp330 as well as some structural and functional measures of properties specific to polarized cellular domains.

Task Significance:

Endocytosis by epithelial cells of the renal proximal tubule serves to reabsorb and degrade the proteins that have escaped the glomerular filter, as demonstrated for a number of proteins. This specialized activity, "degradative endocytosis," is associated with a high turnover of plasma membrane which entails very efficient recycling carried out by specialized structures - the dense apical tubules. Understanding of this process is key to defining mechanisms of toxicity of common nephrotoxins from the polybasic aminoglycoside antibiotics through myeloma light chains. A cell culture model expressing the receptors for these and other toxins will greatly enhance studies of renal toxicity of pharmaceuticals.

Progress During FY 1996:

Renal cortical cell mixture in co-culture: evidence for differentiation**a. Structural Differentiation**

Rat and human renal cortical cells were grown in culture in rotating-wall vessels using stirred fermentors and permeable-bag, traditional 2-D cultures as controls.

The rotating-wall vessel is conducive to vigorous cell growth, as evidenced by the high rates of glucose and oxygen consumption. Seeded at 50,000 cells/ml, rat renal cortical cells reduce glucose in the medium 30mg/dl/day. Alamar blue analysis of cell growth suggests the cells number doubles every 4-6 days.

Structural analysis of human renal cortical cells using semi-quantitative morphometric analysis of 50 grids of images of human renal cortical cells grown under various conditions for 16 days provides evidence for differentiation in the rotating-wall vessel and suggests that the cells differentiated better as a co-culture of the normal renal cortical mix of cells, compared to highly purified proximal tubular cells in culture. The number of microvilli per field was 2 ± 1 in conventional 2-D cultures, 10 ± 4 in 99% pure proximal tubular culture in rotating-wall vessel, 35 ± 11 for the normal cortical cell mix in rotating-wall vessel, and 53 ± 17 in the native human renal cortex. This data suggests not only that microvilli lost in conventional culture reform in the rotating-wall vessel, but that a co-culture of the natural mixture of cells in the renal cortex differentiates better than a pure culture of proximal tubular cells.

b. Expression of highly specialized scavenger pathway receptors implicated in nephrotoxicity

Expression of the giant glycoprotein receptors central to proximal tubular toxicity gp330 (megalin, the Heymann antigen or "gentamicin receptor") and gp280 (the myeloma light chain receptor) which are lost in other forms of cell culture are restored in the rotating-wall vessels.

Analysis of protein expression in cultured cells by antibody binding used classic serial log dilution antibody curves. An increase in binding with a decrease in dilution is pathognomonic for specific antibody binding during flow cytometry analysis. Binding of anti-gp280 or anti-gp330/megalin antisera to membrane vesicles prepared from renal cortical cells after 16 days in culture, detected by the fluorescence of a phycoerythrin tagged secondary antibody, shows an almost one hundred fold increase in binding with antibody dilution pathognomonic of specific binding. This increased gp280 antibody binding in the cells grown in the rotating-wall vessel (STLV) is more than five times the expression seen in stirred fermentors. There was no detectable expression in the conventional cultures. Binding of normal serum and minimal dilution of primary antisera were not detectably different.

After the endosomal pathway had been implicated to play a central role in the function and pathophysiology of these receptors and channels, we were interested to colocalize the entrapped endosomal marker with receptor and channel antibody binding. In this manner, gp280 and gp330/megalin were demonstrated to traffic into the endosomal pathway of renal cells grown in rotating-wall vessel culture.

This data suggests that growing human and rat renal cells in rotating-wall vessels provides a novel model for studies of the most common forms of clinical nephrotoxicity, as this is the only cell culture model which expresses the scavenger pathway receptors gp280 and gp330/megalin.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 9/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-23-01-29

NASA CONTRACT NO.: NAG9-811

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Hammond, T.G., Majewski, R.R., Galvan, D.L., and Lelkes, P.I. De novo expression of aminoglycoside and myeloma protein receptors in renal proximal tubular cells grown in simulated microgravity: a new model for pharmacological protection studies. *In Vitro Cell & Dev Biol.* 32:44A, (1996).

Hammond, T.G., Majewski, R.R., Kaysen, J.H., Goda, F.O., Navar, G.L., Pontillon, F., and Verroust P.J. Gentamicin Inhibits Rat Renal Cortical Homotypic Endosomal Fusion: Role of megalin. *Am J Physiol*, (In Press).

Hammond, T.G., Majewski, R.R., Pontillon, F., Verroust, P.J., Goodwin, T.J., Paddock, S.W., Galvan, D.L. and Lelkes, P.I. H⁺ATPase dependence of "degradative pathway" endosomal fusion. (Submitted).

Excitable Cells and Growth Factors under Microgravity Conditions

PRINCIPAL INVESTIGATOR: Dr. Charles R. Hartzell

Alfred I. duPont Institute

CO-INVESTIGATORS:

Schroedl, N.
Gonda, S.Alfred I. duPont Institute
NASA Johnson Space Center (JSC)

Task Objective:

Peptide growth factors are intimately involved in the regulation of many physiological processes in mammalian, striated muscle. These processes include 1) hyperplastic growth, 2) differentiation, 3) hypertrophic growth, 4) tissue adaptation, 5) the onset and force of contraction, and 6) recovery from damage. Invaluable insights into the mechanisms by which growth factors affect these processes have been gained through studies of cultured muscle cells; however, standard methods do not reproduce tissue-like organizations as cells are confined to two-dimensional (2D) surfaces. Recent research has demonstrated that the three-dimensional (3D) arrangement of cells within aggregates is an important determinant of cellular activity and responsiveness, and we have sought to study the effects of growth factors within the context of 3D-tissue-like, muscle-cell cultures. We postulate that the simulated microgravity environment produced within NASA rotating-wall bioreactors will allow the generation of three-dimensional (3D), tissue-equivalent organizations of cells and that these cultures will respond to growth factors in a manner similar to that seen *in vivo* but dissimilar from that seen in 2D cultures.

Task Description:

Using the NASA bioreactor, we will examine the effects of a three-dimensional, tissue-like organization on neonatal rat heart cells and on young adult rat skeletal muscle cells. Due to the absence of a uniform gravitational force, rotating-wall bioreactors allow cells to orient and associate in a three-dimensional suspension culture system. NASA-designed HARV bioreactors will be used to culture cells isolated from rat cardiac ventricles, satellite cells isolated from rat tibialis anterior muscle, and a clonal rat muscle cell line isolated from rat embryos. Once our systems are established, the degree to which the fluid environment of the HARV can be used to generate tissue-like structures will be assessed. Alterations in the tissue formation process induced by fibroblast growth factor, insulin-like growth factor I, thyroid hormone, and transforming growth factor beta will be evaluated.

Task Significance:

The two-dimensional, unit-gravity constraints of conventional cell culture do not optimally model the three-dimensional cytoarchitectural design of the *in vivo* system. Limitations inherent in standard cell culture systems encourage us to continue the development of innovative *in vitro* model systems that are not limited by gravity-induced constraints and that promote the formation of three-dimensional, *in vivo*-like tissue. The development of three-dimensional muscle models is critical to the study of tissue morphogenesis and to the study of the structure/function relationships in tissues and their constituent cells.

Progress During FY 1996:

CARDIAC MUSCLE EXPERIMENTS

As part of an ongoing tissue engineering effort to study the establishment and maintenance of cardiac architecture *in vitro*, isolated neonatal rat heart cells were allowed to reassociate in low-shear, three-dimensional culture in the presence of extracellular support scaffolds and defined media in NASA-designed High Aspect Ratio Vessels (HARVs). The degree to which mixed populations of cardiocytes retained tissue-specific positional information was evaluated by their ability to reestablish tissue-like organization and function. A combination of biochemical and microscopic techniques were used to characterize the tissue-like, three-dimensional cultures, and the degree to which three-dimensional architecture affected *in vitro* cellular responses to thyroid hormone (tri-iodothyronine, T_3) was determined. We found that isolated neonatal rat cardiac cells retained the ability to regenerate elaborate tissue structures *in vitro*, and we observed that the establishment of these structures resulted in an enhanced cellular response to thyroid hormone. Specific results included:

Primary cultures of isolated cardiac cells reformed tissue-like structures *in vitro*. Cardiac cells in HARVs were arranged in three-dimensional space to form layered tissue-like aggregates which, when viewed by scanning or transmission electron microscopy, contained an outer endocardial cell layer followed by a layer of extracellular matrix and an layer of cardiomyocytes attached to the substrate.

Three-dimensional culture of cardiac cells allowed remodeling of the extracellular matrix. The cardiac cells progressively remodeled the extracellular space in HARV-based cultures. Deposition of matrix material between the nascent endocardial and myocardial cell layers was clearly evident in three-dimensional cultures. Such deposition of matrix was not seen in standard two-dimensional cultures which confine the attachment-dependent, contact-inhibited cells to the surface of the tissue culture plate.

In three-dimensional culture, cardiomyocytes aligned along scaffold matrices. The myocytes in HARV cultures formed layers several cells thick in which all the cells aligned parallel to the axis of the support matrix (most notably type I collagen and polyglycolic acid). The result was the formation of directed, multicellular contractile units.

Three-dimensional cultures of cardiomyocytes responded to adrenergic-receptor agonists and antagonists. Similar to standard, two-dimensional cultures of neonatal rat cardiomyocytes, three-dimensional cultures of cardiac cells grown on collagen fibers beat spontaneously and rhythmically. The frequency of contraction was affected by both adrenergic stimulation and blockade indicating that the cultures were able to reestablish adrenergic circuitry in three-dimensional aggregates.

In HARV-based culture, cardiomyocytes formed tissue-like associations and junctions. Based on electron microscopic observations, neighboring myocytes established gap junctions as well as adherens junctions and exhibited an overall ultrastructural organization characteristic of cardiac tissue *in vivo*. In addition, the distribution of cells in the aggregates produced by HARV-based culture resembled the distribution of cells seen *in vivo* — a continuous layer of endocardial cells was found near the medium followed by matrix material and cardiomyocytes toward the support matrix. Our results suggest that cultured cells can be induced to recapitulate the organization of tissue when grown in the HARV bioreactors.

The distribution of organelles in cardiomyocytes differs depending on the type of system used. The organelles of cardiac cells become organized into distinct patterns when cultured using traditional culture — nuclei localize toward the basolateral surface (near the culture dish) and the majority of sarcomeres distribute between the nuclei and the apical cell surface. In a series of electron microscopic studies, we have found that cells cultured in the simulated microgravity environment of the HARV bioreactors have randomly distributed nuclei with sarcomeres equally present toward and away from the support matrix. Our results suggest that the distribution of organelles in cardiac cell culture is directly affected by the orientation of the gravity vector.

Three-dimensional culture resulted in enhanced cellular sensitivity to T_3 compared to two-dimensional culture. *In vivo* cardiac muscle responds to changes in the level of thyroid hormone by altering the expression of myosin heavy chain genes. Cells cultured in HARV bioreactors responded more readily to physiological doses of applied thyroid hormone (T_3) than did traditional two-dimensional cultures. These results demonstrate the importance of multicellular-organization and organelle-distribution as determinants of *in vitro* cardiac cell function.

SKELETAL MUSCLE AND RMO MYOBLAST CELL LINE EXPERIMENTS

In the search for the best skeletal muscle system for use in the HARV bioreactors, both primary cultures of satellite cells and a myoblast cell line (RMO) have been studied. To investigate the formation of three-dimensional architectures in cultures of satellite cells, a culture method originally described by Strohman et al. (*In Vitro Cellular & Developmental Biology*, 26:201, 1990.) was modified for use with rat satellite cells. Research concerning the RMO cell line centered around further characterizing the proliferative and differentiative characteristics of a subclone which was selected based on its ability to form myotubes. The original RMO cell line (Merrill, *In Vitro Cellular & Developmental Biology*, 25:471, 1989) was derived from rat embryonic cells and has not been extensively studied.

Satellite cells reformed tissue-like architectures *in vitro*. Using a culture method modified from Stroham et al., satellite cells were grown on surfaces with low adhesion. Sylgard™ was coated with Matrigel (Collaborative Research) which had been diluted 1/50 with medium, and satellite cells were cultured on the surface. Histological and immunohistological assessments showed that the interior of the constructs was primarily composed of muscle cells and connective tissue. During prolonged periods of culture, the central portion of the three-dimensional constructs became progressively more organized and took on the appearance of distinct muscle fibers surrounded by a connective tissue sheath. These observations suggest that satellite cells were capable of reforming three-dimensional tissue-like architectures *in vitro*, but further work to improve the consistency and reproducibility of the method is required.

RMo-subclone cells proliferated and differentiated into large, multi-nucleate myotubes. When cultured on a variety of substrates, including Matrigel (diluted 1:10 with medium) or tissue culture plastic, RMo cells formed expansive multi-nucleated myotubes. In standard culture, these myotubes were striated and contractile, and the cultures responded to basic fibroblast growth factor, insulin-like growth factor I, and the presence of serum. In HARV-based culture, on the other hand, the rate of RMo cell proliferation was apparently reduced relative to standard tissue culture controls, and the HARV cultures were non-contractile.

The expression of myogenic transcription factors in cultures of differentiating RMo cells resembled that described for satellite cells. In cultures of RMo cells, MyoD was expressed predominantly during proliferation and was down regulated during myotube differentiation. Myogenin (called Myf4 in some species) was detectable in a small proportion of proliferating cells, but was seen in nearly all myonuclei after fusion: MRF4 (also called MYf6 in some species) was not detected until after myotube formation.

Cultures of RMo cells progressed through multiple stages of differentiation. RMo cells expressed multiple isoforms of myosin including embryonic, neonatal, and fast IIB: after the onset of contraction, RMo myotubes also expressed the slow isoform of myosin; however, expression of the slow myosin isoform was inhibited when contraction was blocked by tetrodotoxin. The flow myosin isoform was not seen in the less developed (and non-contractile) HARV-based cultures. In addition, the RMo cultures expressed the epsilon subunit of the acetylcholine receptor. Our results suggest that RMo cells progressed through several stages of differentiation from the initial mononucleated cell culture.

Expression of desmin was not required for myotube formation in RMo cells. Myotubes formed in cultures of RMo cells without the accumulation of detectable levels of the intermediate filament protein desmin. This result was confirmed with two separate monoclonal antibodies (D3 and DER11). In confluent populations of RMo cells, only 0.02% of cells were desmin positive. Desmin, typically used as a marker for cells in the myogenic lineage, is present in all mammalian muscles, and the expression of desmin has been implicated in myofibrillogenesis and the elaboration of the muscle phenotype. It is, therefore, surprising that RMo cells were capable of forming contraction-competent, multinucleated, striated myotubes without accumulating desmin.

NG108-15 CHOLINERGIC NEURONAL CELL LINE EXPERIMENTS

For nerve/muscle co-culture experiments, we have been developing methods to use the neuroblastoma/glioma fusion cell line NG108-15. Cells were obtained from Dr. Marshall Nirenberg at the NIH. These cells can be made to form neurite outgrowth and cholinergic synapses in culture. Unfortunately, the compounds which have been characterized to cause this differentiation (e.g., dbcAMP) also have dramatic effects on skeletal and cardiac muscle. We have sought to devise a method to induce NG108-15 differentiation without altering cAMP metabolism.

Previous work at the duPont Hospital for Children has suggested that ferritroporphyrin IX (FePPIX) improves the condition of primary muscle cultures (see Schroedl, et al., *Am. J. Physiol.*, 1998. Funanage, et al., *J. Cell Physiol.* 141:591-597, 1989, and Akins and Schroedl. *Molec. Biol. Cell*, 4:2251a). In addition, published accounts suggest that FePPIX enhanced neurite outgrowth in cultured mouse neuroblastoma cells (Ishii and Maniatis, *Nature*, 274:372, 1978). In order to develop co-culturing strategies for NG108-15 with muscle cells, we have investigated the effects of FePPIX on NG108-15 differentiation.

NG108-15 cells exhibited enhanced differentiation (neurite outgrowth) when exposed to FePPIX. As expected, the exposure of NG108-15 cells to FePPIX resulted in differentiation and neurite outgrowth.

Co-cultures of NG108-15 cells with RMo cells in the presence of FePPIX did not result in obvious synapse formation. This effect may be related to the aforementioned lack of desmin expression in the RMo cells as desmin has been reported to accumulate at mature neuromuscular junctions. Interestingly, the RMo cells did not respond to the FePPIX as expected from the previous studies of satellite cells and cardiac cells (i.e., there was no elevation in myosin heavy chain expression relative to untreated cells).

SUMMARY

Significant progress has been made toward the realization of the research goals set out in our original research proposal. Our experiments demonstrate that isolated cardiac and skeletal muscle cells retained the ability to form tissue-like structures in vitro. In addition, important results were obtained in several areas: 1) as assessed at both cellular and sub-cellular levels, three-dimensional structure and ultra-structure were reestablished in vitro when primary cardiac cells were cultured in HARV bioreactors, 2) the establishment of three-dimensional cardiac cultures in the HARVs was found to alter cellular responsiveness to thyroid hormone (T_3) such that the HARV-derived cultures responded in a more tissue-like manner to physiological doses of T_3 than did parallel two-dimensional cultures, and 3) RMo cells were found to proceed through a differentiative program in the absence of desmin; desmin is widely used as a definitive marker for cells in the myogenic lineage, and its absence from the otherwise well-developed RMo myotubes is compelling. We will continue to characterize the in vitro establishment of tissue architecture and its relationship to the genesis of tissue function as we proceed with the development of cardiac and skeletal muscle constructs for use in transplantation therapies.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 12/92 EXPIRATION: 11/96

PROJECT IDENTIFICATION: 962-23-01-07

NASA CONTRACT NO.: NAG-656

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Akins, R.E., Schroedl, N.A., Gonda, S.R., and Hartzell, C.R. Neonatal rat heart cells cultured in simulated microgravity. *In Vitro Cellular and Developmental Biology*, (In Press).

Ho, M.L., Molnar, G., Funanage, V.L., and Schroedl, N.A. Myogenic factor expression and quantitation in satellite cells derived from growth rat muscle. *BAM*, 6(3), 145-155 (1996).

Molnar, G., Ho, M.L., and Schroedl, N.A. Evidence for multiple satellite cell populations and a nonmyogenic cell type that is regulated differently in regenerating and growing skeletal muscle. *Tissue and Cell*, (In Press).

Molnar, G., Ho, M.L., and Schroedl, N.A. RMo myoblasts express a mature skeletal muscle phenotype in the absence of the intermediate filament protein desmin. *J. Cell. Physiol.*, (Submitted).

Molnar, G., Schroedl, N.A., Gonda, S.R., and Hartzel, C.R. Skeletal muscle satellite cells cultured in simulated microgravity. *In Vitro Cellular and Developmental Biology*, (In Press).

Determining the Conditions Necessary for the Development of Functional Replacement Cartilage Using a Microgravity Reactor

PRINCIPAL INVESTIGATOR: Prof. Carole A. Heath

Iowa State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objectives of the second year of the project are to determine the effects of different levels of shear stress, continuous and intermittent, on chondrocyte growth and cartilage regeneration in a rotating-wall (microgravity) vessel.

Task Description:

Mechanical forces have been shown to affect the structure of developing cartilage *in vitro*. With the goal of achieving regenerated tissue that is biologically relevant and useful, we will determine the effects of varying the frequency and time course of applied stress(es) and the effects of microgravity on the development process. Isolated chondrocytes, the cells responsible for producing the components of cartilage, will be cultured in a three-dimensional mesh of resorbable polymer in a modified microgravity reactor which can be operated over the range from very low stress to high shear and/or high compression. By mimicking key aspects of the *in vivo* environment, i.e., structure and stress, we will determine the conditions necessary for regenerating functional cartilage *in vitro* from cultured chondrocytes as well as the effects of microgravity on the process.

Task Significance:

The knowledge gained from this project will bring us closer to a treatment for osteoarthritis and other diseases and injuries of the articulating joints and to an understanding of the effects of microgravity, as experienced in space flight, on cartilage development. The generation of an *in vitro*-engineered sheet of replacement articular cartilage, if it can be successfully implanted *in vivo*, would precipitate a revolution in the management of severely impaired dysfunctional joints.

Progress During FY 1996:

Progress to date has included i) investigations of cartilage development (including both cell growth and matrix formation) under intermittent compression at low levels of pressure and ii) design and construction of the modified rotating-wall vessel to allow for continuous perfusion of chondrocyte/polymer composites cultured under different levels of continuous or intermittent shear stress. Studies at higher levels of compression are under way in a device (the construction of which was just recently completed) designed solely for application of a wide range of intermittent compression stresses on the immobilized cells. The first set of experiments were designed to determine the effect of normal (approximately 3 MPa) levels of intermittent compression on cultured chondrocytes. These initial experiments suggest that pressurization results in greater concentrations of cells and sulfated glycosaminoglycans (one of the key extracellular matrix components and which is primarily responsible for maintaining tissue hydration) than the control (unstressed) cell/polymer constructs.

The redesigned rotating-wall vessel (modified for continuous perfusion of cell/polymer pads in collaboration with Synthecon) has finally been completed. We are in the process of setting up experimental studies of chondrocyte culture and matrix formation in porous, resorbable polymer matrices at very low levels of shear stress.

Other experimental variables have also been determined, or are in progress, in preparation for the long-term cartilage regeneration studies. These include i) establishing a protocol for determining the mechanical properties of the regenerated cartilage and comparing those measurements to those of native tissue, ii) determining the effects of different buffer conditions on chondrocyte growth, iii) comparing the growth and matrix formation by chondrocytes harvested from juvenile and adult animals, and iv) evaluating the effects of nutrient concentration on cell growth. All of these variables are important in execution and evaluation of the studies examining the effects of stress on chondrocyte growth and cartilage development *in vitro*.

Plans for the coming year include i) continuation of the compression studies to determine the effects of different levels and frequencies of compressive stress on chondrocyte growth and cartilage development, ii) studies of the effects of different levels and frequencies of shear stress on chondrocyte growth and cartilage development in the modified rotating-wall vessel, and iii) comparison of the effects observed between continuous and intermittent application of shear stress on developing cartilage.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-23-01-34

NASA CONTRACT NO.: NAG9-827

RESPONSIBLE CENTER: JSC

The Effects of Microgravity on Viral Replication

PRINCIPAL INVESTIGATOR: John H. Hughes, Ph.D.

Ohio State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The overall goal of this project is to assess the effects of microgravity on various aspects of viral replication. The specific objectives are:

- 1) To determine viral yields for different viruses grown in different cells at microgravity.
- 2) To determine the effects of either acute or chronic microgravity on the replication of several different human viruses that are grown in different cells.
- 3) To determine if cells latently infected with viruses are activated to produce more virus when grown at microgravity than when the same cells are grown at 1g.
- 4) To determine if viruses that cannot be grown in conventional cell culture systems at 1g can be grown in cells at microgravity.

For comparative and control purposes, viral replication in cells grown at hypergravity and 1g (standard culture) will also be examined.

Task Description:

For this project, we will use a simulated microgravity environment to investigate viral replication. The simulated microgravity environment will be generated by one of the NASA-designed Rotating-Wall Vessels (RWVs). Some key issues to be addressed are whether microgravity plays a role in viral-cell interactions and whether microgravity can affect viral pathogenesis. To study any effects of microgravity on viral replication, both DNA and RNA viruses will be used. For the effects of microgravity on latent viruses, we will test lymphoblastoid cell lines infected with the Epstein-Barr Virus and mouse cell lines infected with retroviruses. Lastly, differentiated cells induced at microgravity will be studied to determine if they will be permissive for the replication of viruses that currently cannot be grown *in vitro*. Viral yields for viruses produced at microgravity and 1g will be determined by plaque assay. For viruses that only replicate *in vivo*, a quantitative polymerase chain reaction will be used to monitor viral replication.

Task Significance:

Information about the replication of infectious agents at microgravity is limited. Our studies are aimed at understanding and determining the effects of microgravity on infected cells. If microgravity can activate latent viral infections, then the activation of varicella-zoster virus and the induction of shingles during space flight could be a significant health problem. Our proposed studies should help determine if microgravity has any adverse effects on latent viral infections.

In the past, virological studies with infected cells have opened new avenues of research involved with cellular functions. Currently, certain viruses such as some hepatitis viruses, wart viruses, etc. will only replicate *in vivo* but not *in vitro*. Since these viruses replicate in differentiated cells *in vivo*, there are obviously some cellular factors that permit their replication or inhibit their replication. Differentiated cells induced at microgravity may provide the critical cell or host-factors needed for the replication of certain viruses. If this is the case, then microgravity conditions could provide a new biotechnology tool for developing control measures (new vaccines and antivirals) as well as allowing for the production of new diagnostic products.

Progress During FY 1996:

Selection of Rhinoviruses for Microgravity Studies. Since information about the replication of infectious agents at microgravity is limited, our studies were aimed at understanding and determining the effects of microgravity on infected cells. A rhinovirus was selected as a pathogenic agent to investigate the effects of

microgravity on viral replication. For our studies, HeLa cells were used. Prior to infecting with the virus, cells were maintained in 3-dimensional (3D) cultures on microcarrier beads at microgravity in RWVs or in Teflon bottles at 1xg for a minimum of 5 days and as long as 19 days for one experiment.

Establishment of Appropriate Control Conditions. Teflon bottles were selected as vessels for control cultures. Conventional plastic or glass roller bottles do not allow the 3D cultivation of cells on microcarrier beads. Cells growing on beads adhere to the walls of the roller bottle and grow as monolayers. However, rotating Teflon bottles having constant motion and little turbulence permitted the growth of cells on beads in 3D cultures. Teflon bottle cultures proved to be an effective control, comparing favorably to RWVs both in total numbers of cells and overall cell viability.

Experimental Design. Viral infections were carried out with a multiplicity of infection (MOI)<1.0. A low MOI was used because it permitted infections to be followed over a period of 5-6 days at microgravity conditions. If high MOIs were used, all cells would have been infected and killed within 10 hours, and, consequently, any impact due to microgravity may not have been readily observed.

One growth cycle for rhinovirus replication takes 10-16 hours. The new virus can be detected intracellularly 5 to 6 hours. Samples were collected from RWVs, Teflon bottles and tissue culture flasks at 3, 8, and 10 hours. These time points were selected in order to provide information about viral adsorption at 3 hours, while 8 and 10 hours provide data on release of new virus after one cycle of viral replication. In addition, after multiple cycles of viral replication, samples were also collected for viral assay.

Results and Discussion. Our results indicate that significantly less virus was present in the supernatant of RWV cultures at 3 hours as compared to cultures in Teflon bottles. Additionally, 3 hours following infection, significantly less virus was present in total viral samples (samples containing cells and supernatant) from RWVs as compared to samples from Teflon bottles. Thus, not only was there less free-virus remaining in the supernatant at that time, but less cell-associated virus as well. This could be the result of cells grown in microgravity being better able to absorb and internalize virus, or the physical conditions existing within the RWV may allow for more efficient interaction between cells and virus.

An interesting observation was that significantly less virus was present in the supernatant of tissue culture flasks with monolayers at 8 hours as compared to in both RWVs and Teflon bottles. By 10 hours there was no difference between the amount of virus found in supernatant tissue culture fluids from RWVs and Teflon bottles or tissue culture flasks. However, at this time, RWVs and Teflon bottles had 2.9 and 2.4-fold more virus respectively than that found in tissue culture flasks. This indicates that cultivation of cells under conditions with motion results in a more rapid replication of virus, possibly shortening the time required to complete a single growth cycle. Previous reports have indicated that motion can enhance rhinovirus yields and cytopathic effects (Reviewed in Clin. Micro. Rev. 6:150, 1993).

Since one growth cycle for rhinoviruses takes approximately 10 hours, sampling at 21 hours post-infection gave information on viral yields after two replication cycles. At this time point, viral yields (total virus samples) from microgravity cultures were significantly higher (2.2-fold) than those obtained from cultures grown at 1xg in a Teflon bottle. This observation was made in each of 3 independent experiments. In addition, at 5 and 6 days post-infection, significantly more virus (9 and 12-fold respectively) was present in RWVs than was present in Teflon bottles.

An explanation of the differences in viral yields that we have observed between infected cultures at microgravity versus at 1xg may be due to culture conditions and not microgravity. For example, culture conditions that were different between RWVs (microgravity) and Teflon bottles (1 xg) were zero head space and gas tension (O_2/CO_2) in the RWVs. Currently, we cannot conduct equivalent studies at 1 xg because it is not possible to run long-term studies in sealed Teflon bottles with zero head space. Consequently, because of differences in technology between RWVs versus conventional cell culture methods, gas tension and head space cannot be adequately controlled at this time. When we compared, in a single experiment, viral replication using mature monolayers in T-flasks at various gas tensions, no significant differences in viral yields were detected. We did control for the 3D organization of cells at microgravity and at 1 xg. Therefore, the increase in viral yields we noted at microgravity were not due to 3D versus 2D conditions because all cultures were at 3D.

Additional Studies. Experiments are currently in progress to investigate the effects that microgravity may have on latent viral infections (Objective 3). Furthermore, for control purposes, acute, low-level hypergravity conditions are being evaluated for their effects on viral replication. So far, hypergravity (1.9 xg) significantly enhances the proliferation of cells. Enhanced cellular proliferation at hypergravity may make cells more permissive for certain viruses.

Conclusions. Our results indicate that rhinovirus replication appears to be significantly enhanced at microgravity conditions within RWVs. Cultivation of cells under conditions of microgravity possibly affects the rate of viral adsorption/uptake, the viral replication cycle, and/or viral yield. Finally, the RWVs have proven to be an effective means for culturing human rhinoviruses.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-23-01-26

NASA CONTRACT No.: NAG9-818

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Hughes, J.H., Pierson, S., and Long, J.P. "The Effects of Microgravity on Viral Replication." NASA Biotechnology Conference, Houston, TX., February 23-24, 1996.

Sensitized Lymphocytes for Tumor Therapy Grown in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Marylou Ingram

Huntington Medical Research Institutes

CO-INVESTIGATORS:

Techy, G.
Saroufeem, R.
Narayan, S.
Yazan, O.
Goodwin, T.

HMRI
HMRI
HMRI
HMRI

NASA Johnson Space Center (JSC)

Task Objective:

The NASA High Aspect Ratio Vessel (HARV) bioreactor is used to generate spheroids of human tumor cells. These spheroids are then used to sensitize the patient's lymphocytes to the patient's own tumor. The population of tumor-sensitized lymphocytes (TSL) is then expanded in culture in the presence of interleukin-2 (IL-2) and used in immunotherapy of the patient. *In vitro* studies of the cell biology of tumor cells and cells of tumor stroma cultured in simulated microgravity are an important component of the research.

Task Description:

This is a small scale, in depth pilot study in which nonspecifically stimulated autologous lymphocytes (ASL) and tumor-sensitized lymphocytes (TSL) are administered serially by intralesional injection as local immunotherapy of invasive carcinoma of the urinary bladder. This is a modification of cellular immunotherapy that we have applied with encouraging results in clinical trials to treat recurrent malignant gliomas (Ingram, M., Buckwalter, J.G., Jacques, D.G., et al. Neurological Research 12:265-273 (1990)). For the bladder cancer, the urological surgeon will inject cells intralesionally at intervals of approximately three weeks. Response to therapy will be determined by direct observation of the lesions, serial biopsies for histological and cytological studies, clinical evaluations, and radiological exams. The ability to biopsy lesions at various times after injection of stimulated immune cells is an important advantage in understanding response to therapy and in refining the therapy. The pilot study provides an opportunity to evaluate the NASA HARV bioreactor as a method for culturing tumors as spheroids as contrasted with conventional monolayer cultures. Tumor spheroids *in vitro* have a number of characteristics present *in vivo* but absent from monolayer cell cultures. These characteristics, some of which will undoubtedly be important in the generation of TSL cells, include the presence of specific tumor markers, angiogenesis and growth factors, biological response modifiers, gap junctions, and tumor suppressor gene expression.

Task Significance:

Cancer of the urinary bladder is of special interest in immunotherapy because it has already been shown that immunotherapy in the form of BCG treatment is efficacious. It is now widely used in clinical management of invasive bladder cancer. Thus, there is sound evidence that appropriate mobilization of the patient's own cellular immune mechanisms can have therapeutic efficacy. A number of investigators have recognized the possibility that TSL may offer significant advantages in adoptive immunotherapy, and there has been a recent resurgence of interest in this approach (Greenberg, P.D., Riddell, S.R.J., Natl. Cancer Inst. 84: 1059-61 (1992)). TSL can be expected to show increased tumor cell killing, as do tumor-infiltrating lymphocytes (TIL), and they also hold forth the promise of serving as probes for identifying immunogenic gene products in the tumor.

Many elderly patients with multiple tumors of the urinary bladder cannot tolerate extensive surgery or extensive chemotherapy and may either have failed to respond to BCG immunotherapy or are too unwell to tolerate side effects of that therapy. These patients present a frustrating therapeutic problem to the urologist. We believe that local immunotherapy would be well tolerated by these patients and that it is a rational therapeutic strategy. A clinical trial of this therapy will also provide valuable information about how stimulated immune cells select and identify their target cells, how they migrate through tissue, whether or not they continue to proliferate after injection, and other important considerations that will advance our understanding of cellular immunotherapy and aid in refining it for treatment of bladder cancer and ultimately other cancers.

At the cellular level, the studies can be expected to provide new information about tumor cell biology, especially interactions among tumor cells and stromal cells, including cells of the microvascular and immune systems.

Progress During FY 1996:

During FY 96 we have expanded the set of human tumor cell lines cultured successfully without carrier beads in the HARV bioreactor. All of these cell lines are otherwise anchorage dependent. Cultures are initiated with a monodisperse suspension containing 1-2 million cells per ml of nutrient medium and are maintained for periods of a few days to approximately a month. The spheroids produced are fixed in Carnoy's/Bouin's fixative, then sectioned and stained. Some sections of each specimen are stained with hematoxylin and eosin and other sections from the same specimen are stained immunohistochemically to demonstrate various markers of interest.

When cultured in the bioreactor, each cell line produces spheroids that demonstrate cell line-specific microscopic architecture. Thus, gliomas tend to form small, compact spheroids that sometimes fuse to form larger bodies; the PC3 cell line that was developed from prostate carcinoma metastatic in bone forms discrete spheroids in which cells are very loosely associated. Another prostatic carcinoma cell line, LNCaP, typically forms elongated tubule-like or folded structures. The bladder carcinoma cell line, HBL2, that we recently developed, shows a definite tendency towards epithelial differentiation. The tendency for the HBL2 cells to assemble in such a pattern suggests that various cell adhesion molecules play a role in determining spheroid morphology. Immunohistochemical staining to demonstrate fibronectin, collagen, vimentin, CD44, and other cell adhesion molecules can be expected to provide further insight into spheroid formation and differentiation. So far, we have found cytokeratin, CD44 and E cadherin to be definitely up-regulated in spheroids as contrasted with monolayer cells.

Our clinical collaborator has provided additional surgical specimens of bladder tumors, and these have been invaluable. They have allowed us to refine tissue culture methods specifically for bladder cancer, and two of the specimens have yielded cell lines.

The clinical trial of immunotherapy of bladder cancer has been interrupted due to illness of our clinical collaborator, hence no new patients have been treated. Extension of the IND (BB IND #5163) for the trial has been requested from the U.S. Food and Drug Administration and from Amgen, the supplier of recombinant human interleukin-2 for the study. During the hiatus in the clinical trial, we have concentrated on the *in vitro* research components that may be summarized as follows:

We have extended the list of tumor cell lines as well as stromal cell lines cultured without carrier beads in simulated microgravity, with special attention to cells from new surgical specimens. This is important because cells recently isolated from clinical specimens are more like tumors *in vitro* than are long-established cell lines. Early passage cells lines developed at Huntington Medical Research Institutes and cultured in the HARV bioreactor include 1) breast cancer lines, BRS3 (1st) and BRS10 (2nd), 2) bladder cancer lines, HBL2 (6th) and HBL27 (6th), 3) urothelial cancer, HUC 1 (5th), 4) prostate cancer, PC3 (6th) from cryopreserved specimen, 5) gliomas, HBR 9 (8th), HDBR 147 (8th), 6) HBR 51 (9th), HBR 65 (9th), HBR 84 (7th), O1 T (7th), OT 2 (5th), and 7) metastatic brain tumor, HBM 10 (5th) fibroblasts from BRS 3 (5th) and BRS 10 (4th) and normal prostate fibroblasts, NPF 209 (4th). Three-dimensional structures produced in these cultures have been compared with monolayer-grown cells that have been harvested and centrifuged into a pellet before fixation. Sections of the cultures are stained with hemtoxylin and eosin and duplicate sections are stained immunochemically to identify gene products of interest.

Simulated microgravity culture technology is proving remarkably advantageous for studying interactions of one cell type with another in co-cultures. We are currently exploiting this capability not only to investigate interactions of immune cells with autologous tumors but also to study the interactions of tumor cells and stromal cells. For example, suspensions of malignant epithelial cells (bladder, prostate or breast cancer), when added to small (4 day) preformed spheroids of fibroblasts, demonstrate intrinsic properties that are not manifest when the cells are cultured alone in the bioreactor. They form epithelium-like layers on the fibroblast spheroids and also invade the spheroids. The profound influence of the epithelial cells on fibroblasts is well illustrated in co-culture specimens that are stained immunochemically to demonstrate the presence of tenascin, an extracellular matrix glycoprotein produced by embryonic mesenchme but not by fibroblasts in fully differentiated tissue. It has been demonstrated that malignant epithelium, like epithelium in the embryo and during wound healing, induces the production of tenascin by the underlying fibroblasts. Tenascin, in turn, may stimulate growth of the epithelium. Recently it has also been shown that tenascin is a general immunosuppressive molecule that interferes with T cell receptor/CD3-dependent

signal transduction in T cell activation. In the co-cultures referred to above, when malignant epithelial cells form an epithelium-like layer on normal fibroblasts, they do induce the expression of tenascin, an observation of substantial potential significance in tumor immunology. The co-culture results also suggest that simulated microgravity culture technology will be of considerable value in assaying invasive properties of malignant epithelium, endothelium, immune cells, and other cells of interest.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 11/92 EXPIRATION: 11/95

PROJECT IDENTIFICATION: 962-23-01-14

NASA CONTRACT NO.: NAG-649

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Ingram, M., Techy, G.B., Saroufeem, R., Yazan, O., Narayan, K.S., Goodwin, T., and Spaulding, G.F. Three-dimensional growth patterns of various human tumor cell lines in simulated microgravity of a NASA bioreactor. *In Vitro J. Soc., In Vitro Biol.*, In Press, (1996).

PRINCIPAL INVESTIGATOR: Dr. J. M. Jessup

New England Deaconess Hospital

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this project is to test the fidelity with which microgravity models three-dimensional tissues by assessing how well microgravity affects the molecular and biological function of MIP-101, a human colorectal carcinoma.

Task Description:

MIP-101 is a poorly differentiated adenocarcinoma of the colon that was derived from the ascites of a patient who had widespread metastases within the abdominal cavity. MIP-101 cells are grown in the rotating wall vessel (RWV) with or without normal host cells and assessed for the production of carcinoembryonic antigen (CEA — a 180 kDa glycoprotein that is produced by carcinomas and used clinically as a tumor marker) and for biological behavior including adhesion and metastasis. Cells grown in microcarrier bead cultures in the RWV under simulated microgravity are compared to similar MIP-101 cultures grown on microcarrier beads in stationary culture as well as in conventional monolayer cultures.

Task Significance:

One of the prime goals of the biotechnology program at NASA Johnson Space Center is to determine whether cultivation of cells in microgravity produces three-dimensional cultures that mimic the morphology and function of tissues in living animals or humans. The MIP-101 cells are an excellent test of this because they are poorly metastatic in experimental models of metastasis in athymic nude mice and do not produce CEA in conventional monolayer culture systems. We have shown that CEA injected into mice enhances production of liver metastases by MIP-101 cells and that MIP-101 cells will metastasize when implanted into the abdominal cavity after producing CEA. MIP-101 cells placed in the subcutaneous tissue of the mouse do not metastasize and do not produce CEA. Furthermore, cells grown on plastic or conventional substrates such as Matrigel or laminin are neither metastatic nor induced to produce CEA.

The conventional interpretation of these results is that the microenvironment (the three-dimensional environment) of the abdominal cavity induces MIP-101 cells first to produce CEA and then to develop blood-borne metastases in the liver and lungs of nude mice. Early experiments in the RWV question this conventional interpretation of the effects of host microenvironment because they demonstrated that CEA production may be induced in MIP-101 cells when they are grown in the RWV in the absence of any abdominal cavity stromal cells. This suggests that the MIP-101 cells may produce CEA when they are allowed to grow in three dimensions. Thus, the absence of CEA production in subcutaneous tumors is due to an inhibition of CEA production by the subcutaneous tissue rather than promotion of CEA production and metastatic potential by the abdominal cavity.

This system is an excellent model in which to test the fidelity of the RWV culture system because the first stage in metastasis by MIP-101 cells appears to be the induction of CEA production, followed by the acquisition of the ability to develop experimental metastases after injection into the spleen of nude mice. Assessment of fidelity of the RWV culture system is simplified by first testing for the production of CEA, tumor marker, then assessing the biological aspects of metastasis.

Progress During FY 1996:

The primary goal of the Biotechnology Program at NASA Johnson Space Center is to determine whether cells cultivated in microgravity produce three-dimensional cultures that mimic the morphology and function of tissues in living humans or animals. Hopefully, the culture system will permit the creation of three-dimensional structures that may either product novel molecules such as growth factors or which may be used for reimplantation into patients. We have used the MIP-101 cell line to study the usefulness of the Rotating Wall Vessel (RWV) as a bioreactor. MIP-101 is a poorly differentiated human colon carcinoma cell line that in monolayer culture in vitro

Discipline: Biotechnology

... 180-200 kDa CEA molecule is increased 1.5 to 2.5-fold over the ... is exciting because CEA expression may be related to the ability of human colon carcinoma cells to metastasize.

When we examined these MIP-101 cells growing in the RWV for NCA expression, we found that both NCA50 and NCA90 protein was expressed and that like CEA, the protein expression was increased in RWV cultures but to a greater extent. Usually, the increase in NCA expression was 5 to 8-fold over monolayer culture. Growth in stationary three-dimensional spheroids also increased the expression of NCA and CEA to almost as high levels.

When we analyzed the gene transcripts for CEA and NCA, we were surprised to find that there is almost no CEA mRNA produced compared to NCA. The monolayer cultures do not produce detectable CEA mRNA, and the cells cultured in the RWV produced approximately 0.001 attomoles of mRNA. Thus, the increase in the expression of CEA protein may be used to increase protein stability since there does not appear to be an increase in mRNA. Interestingly, the NCA mRNA was increased 40-fold in the RWV cultures since quantitative RT-PCR demonstrated only 0.001 attomoles of NCA mRNA in monolayer cultures and 0.04 attomoles of NCA mRNA in the RWV cultures. This is important because it has been recently appreciated that NCA upregulation may be even greater than that of CEA during colonic neoplastic transformation. The regulation of protein stability is an important issue that is currently under study, and that will be the focus of the next year's work.

STUDENTS FUNDED UNDER RESEARCH:	TASK INITIATION: 1/93	EXPIRATION: 1/97
	PROJECT IDENTIFICATION: 962-23-01-13	
	NASA CONTRACT No.: NAG-650	
	RESPONSIBLE CENTER: JSC	

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Jessup, J.M., Brown, D., Fitzgerald, W., Ford, R.D., Nachman, A., Goodwin, T.J., and Spaulding, G. Induction of Carcinoembryonic Antigen Expression in a Three-Dimensional Culture System. *In Vitro Cell Biol Develop.*, (In Press).

Use of Rotating Wall Vessel (RWV) to Facilitate Culture of Norwalk Virus

PRINCIPAL INVESTIGATOR: Dr. Philip Johnson, M.D.

University of Texas Medical School at Houston

CO-INVESTIGATORS:

Oefinger, P.

SciCor Laboratories, Indianapolis, Indiana

Task Objective:

The objective of the project is to use the NASA-developed slow-turning lateral vessel (STLV), a type of rotating-wall vessel (RWV) used for differentiation of tissue cultures, to facilitate culture of Norwalk virus. We will culture and confirm differentiation of various human intestinal cell lines or populations. With this completed, stool specimens derived from Norwalk virus-infected volunteers will be used to infect selected human intestinal cell lines obtained from RWV tissue culture differentiation studies. The infected cell cultures will be characterized for evidence of Norwalk virus replication by immunochemical, biochemical, ultrastructural, histological, and infectivity studies, and neutralization assays. Finally, we plan to generate tissue culture adapted strains of Norwalk virus with enhanced replication properties in conventional tissue culture lines and systems.

Task Description:

This project will use the RWV as a means to develop a tissue culture system for Norwalk virus, a gastroenteric pathogen. In collaboration with Dr. M.P. Moyer and T. Goodwin, we have gained the expertise of tissue culture establishment of human intestinal-derived cell populations in the RWV system. This system is being refined for our purpose of propagating Norwalk virus. The project utilizes the collected specimens from our human volunteer Norwalk virus-challenge studies as an inoculum. Evidence will be accumulated, as discussed in objectives, to confirm replication of the virus in the RWV system. Once samples enriched for putative progeny virus populations have been identified, further characterization of the material will occur. These include gradient purification, biochemical analysis, and electron microscopy. As a conclusive test, the progeny virus from the cultures will be passed several times into new RWV cultures. The confirmation of replication of the Norwalk virus will be undertaken as occurred previously with the primary passages. Eventually, the RWV-derived Norwalk strains will be adapted to conventional culture systems, which will enable tests such as neutralization assays to be performed to evaluate the immunogenic efficacy of future Norwalk virus vaccine preparations.

Task Significance:

The successful propagation of the Norwalk virus may require a differentiated intestinal tissue culture system. A well-known Norwalk virus inoculum, 8Flla, is infectious in human volunteer studies, but has not been demonstrated to replicate in vitro. Approximately 60% of volunteer individuals challenged with Norwalk virus do experience gastroenteritis, corroborated with studies at this institution by us. Disease occurs in the upper small intestine. Since the original inoculum used for human volunteer studies is being depleted, other sources of infectious virus need to be generated for studies in basic virology, vaccine development, and infectious dose volunteer challenge studies. It is our contention that mature three-dimensional cultures of human intestinal tissue will support Norwalk virus growth, whereas undifferentiated or unrelated tissues are inadequate to do so. Progeny viruses generated by these studies will be used in future testing of vaccine trial efficacy through demonstration of neutralizing antibodies of immunized individuals.

Progress During FY 1996:

One of the first well-documented confirmations of the enhanced tissue culture system provided by the RWV was reported by Goodwin, Moyer, and coworkers, (P.S.E.B.M., 202: 181, 1993). Human mesenchymal cells were established on microcarrier beads in the RWV, followed by the addition of small intestinal epithelial cells. The cell cultures developed into a three-dimensional array containing differentiated cellular markers that were not detectable or lowly expressed in conventional monolayer cells. Their report exemplifies the possibility of completely new aspects of biological investigations, including applications in the private sector.

In collaboration with Dr. Mary Pat Moyer at the University of Texas Health Science Center at San Antonio, we initiated pilot studies to propagate the Norwalk virus. We have preliminary evidence that the Norwalk virus can be

cultured utilizing this system. Using the cell preparations reported in her article, we infected these and other cultures with a Norwalk inoculum derived from human volunteer studies.

Preliminary ultrastructural analysis of these mesenchymal/epithelial human intestinal cells infected with the Norwalk virus was undertaken. At day 0 prior to infection, the ultrastructure appears without obvious pathology. However, at day 6 post-infection, cytoplasmic vacuoles are noted. This pathology progressed to frank cytoplasmic degradation and nuclear condensation by day 8 post-infection.

Immunohistological staining of Norwalk-infected formalin fixed and paraffinized tissue from the RWV has been pursued. Acute and convalescent (≥ 3 weeks after illness) paired sera from two of our Norwalk-challenged volunteer donors as well as hyperimmune rabbit anti-recombinant Norwalk virus (rNV) capsid serum (supplied in collaboration by Dr. M.E. Estes) have been used in an immunoperoxidase staining and ELISA procedures.

Our further studies support the contention that there is some level of Norwalk virus replication in the human mesenchymal/epithelial cells grown in the RWV. Low levels of detectable antigen by solid phase and *in situ* immunochemistry were noted in these cultures. In addition, glucose consumption fell during days 6 and 8 post-infection. The evidence of Norwalk virus replication within the primary human intestinal cell cultures grown in the RWV was quite encouraging. However, the difficulty and reliability in obtaining these primary cell populations has necessitated a search for alternative tissue culture sources. Accordingly, we have been investigating several established human intestinal cell lines for adaptation within the RWV.

Prior to beginning culture of the human intestinal cell lines in the RWV, several quality control aspects had to be addressed for the project. A proven source of intact Norwalk virus particles has been identified. The sample used for partial cloning of the Norwalk virus genome (co-author P.C. Johnson, J. Clin. Invest. 87:1456-1461, 1991) has been confirmed by immune-electron microscopy to contain Norwalk virus particles, as aggregated with the hyperimmune rabbit serum against rNV (supplied by Dr. M. Estes). Additionally, the immunoperoxidase reactivity of the rabbit anti-rNV established with SF9 cells secreting rNV from the baculovirus expression vector has been confirmed. The immunostaining of these paraffinized- or cytospin-prepared cells can be blocked with hyperimmune serum that is absorbed with purified rNV. We have also learned that acetone is the best fixative for maintenance of the intracellular Norwalk antigen immunoreactivity.

As a prototype experiment, several human intestinal tissue culture cell lines were established in a culture on microcarrier beads in the RWV. At two weeks of culture, the cells were beginning to cover the microcarrier beads as seen by phase contrast microscopy. Evidence of three-dimensional structure was evident. Initial differentiation studies have detected keratin within these microcarrier RWV cultures. The cells appear to be arranging themselves in a pattern similar to gut epithelium.

The search for an optimal human intestinal cell line is ongoing for our purpose of Norwalk virus culture. Initial studies have been encouraging. Samples were harvested daily for the first four days after infection and every other day thereafter. Using hyperimmune sera, obtained from immunized animals with rNV capsid stocks, infected cells were analyzed for evidence of Norwalk virus replication. Cell samples were fixed in formalin and paraffinized for immunochemical analysis. Cytoplasmic reactivity was noted in rare cells within one day post-infection. The total number of cells displaying immunoperoxidase reactivity was found to increase several-fold with cell samples from subsequent days post-infection. The immunostaining reactivity is blocked when the hyperimmune serum is preincubated with rNV capsid preparations, supplied by Dr. Mary Estes. Borderline levels of Norwalk virus were detected by the polyclonal anti-rNV ELISA, but these samples were negative by PCR. The histological and ultrastructural investigation of this work is currently being evaluated.

Unexpectedly, the individual human intestinal cell lines that have been tested in the RWV appear to enter early senescence. This fact was also corroborated at the NASA Investigators Working Group (IWG) meeting held earlier this year in Houston. As a result of this conference and our observations, we recently convened our collaborators together in a planning session. Dr. Moyer has established two separate fibroblast and epithelial cell lines of intestinal origin. Our plan is to recreate the matrix environment resulting from coculture of fibroblast and epithelial cells that occurred in the original primary intestinal cell RWV culture. The hypothesis is that the longevity of the epithelial cells will be lengthened due to this coculture system, thereby allowing progeny Norwalk viruses to replicate more efficiently in the RWV cultures. We are currently culturing these cells from Dr. Moyer's laboratory,

II. MSAD Program Tasks — Ground-based Research

Discipline: Biotechnology

and we will later initiate RWV infection experiments. If these experiments do not prove as promising as those generated with primary cells, we will eventually resort to primary cell usage to generate a tissue culture-adapted strain of Norwalk virus.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-23-01-31

NASA CONTRACT No.: NAG

RESPONSIBLE CENTER: JSC

Fibril Formation by Alzheimer's Disease Amyloid in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Daniel A. Kirschner

Boston College

CO-INVESTIGATORS:

Inouye, H.
Malinchik, S.

Boston College
Boston College

Task Objective:

In working towards our overall goal of microgravity-assembly of A-beta fibrils, we will first undertake appropriate ground-based experiments to gain further experience in working with the full-length amyloid peptides and to develop from neutron diffraction measurements additional structural constraints for modeling the subunit organization of the amyloid fibril.

Specific Aim (1): To generate oriented fibrillar assemblies of the A-beta peptides that are most relevant to understanding amyloid formation, structure, and toxicity.

Specific Aim (2): To pursue questions about A-beta assembly and structure stimulated by recent results in the field.

Specific Aim (3): To further develop molecular models for A-beta fibrils based on additional structural constraints imposed by the improved x-ray data and new neutron diffraction data.

Task Description:

Our previous experiments mainly utilized peptide fragments corresponding to the putative extracellular domain of amyloid-beta, although some 40-mers were studied (primate, rodent, and Dutch-haemorrhagic analogues). The difficulty in undertaking fiber diffraction from 40-mer samples is that, unlike most of the shorter peptides, the assembled fibers do not easily orient in a magnetic field, which results in more overlap among the x-ray reflections, in turn making the diffraction patterns considerably more difficult to interpret. However, considering the preponderance of the 1-40 and 1-42 amyloid proteins in AD tissue, we are focusing our fibrillogenesis efforts on these full-length peptides. Obtaining well-oriented fibers and interpretable x-ray patterns will have important bearing on our subsequent molecular modeling.

Task Significance:

In Alzheimer's disease, a normally-occurring protein termed beta-amyloid accumulates between the nerve cells. The formation and accumulation of this material profoundly affects the functioning of the central nervous system, as amyloid can be neurotoxic. To characterize the mechanism by which the amyloid forms and exerts its effects, we have been studying fibrillogenesis using the tools of structural biology (x-ray fiber diffraction, electron microscopy). A detailed understanding of the three-dimensional organization of amyloid will complement the information currently being obtained from analytical protein chemistry and immunocytochemistry, and more recently from light scattering and magnetic resonance, and will provide valuable insights into the pathogenesis of pre-amyloid deposits, neuritic plaques, and cerebrovascular amyloid. By establishing the molecular organization of amyloid, we hope to provide a rationale basis for developing agents for diagnostic imaging of the deposits and therapeutics for preventing or arresting fibrillogenesis.

Progress During FY 1996:

1. "Dry drop test." Owing to the high cost of synthetic peptides and our need to survey a variety of conditions for peptide assembly and orientation, we have sought to develop a method that utilizes microgram quantities of peptide for screening. We found that monitoring the birefringence of a dried peptide solution could supply information about aggregation properties of beta-amyloid fibers. Thus, a 0.5 microliter drop of beta-amyloid solution at concentration of 1-10 mg/ml is allowed to dry on a siliconized glass surface. The protein tends to concentrate along the circular order of the liquid-glass interface. Birefringence of the circular area is checked by a polarizing microscope. To understand the relationship of aggregation properties of beta-amyloid and the degree of birefringence found in the dry drop, we tested different beta-amyloid fragments, and compared results with the gallery of x-ray

diffraction patterns from different beta-amyloid fragments (Inouye *et al.*, 1993). Analysis of the x-ray diffraction patterns of A-beta(11-28), A-beta(13-28), A-beta(11-25), A-beta(9-28) and A-beta(19-28) amyloid fragments revealed a positive correlation between the "crystallinity" of samples oriented in a magnetic field and the degree of birefringence of the dried drop of the corresponding peptide solution.

2. The use of salts to induce lateral aggregation of beta-amyloid fibers. We have previously found that in the presence of sulfate ions, fibrillar assemblies of A-beta fragments undergo extensive lateral aggregation. Since such aggregation may be crucial in orienting A-beta(1-40) we explored the influence of sulfate ions on aggregation properties of this fragment. Sodium sulfate (Na_2SO_4) and ammonium sulfate ($(\text{NH}_4)_2\text{SO}_4$) at concentrations of about 40 mM were found to cause extensive precipitation of the A-beta(1-40), likely due to "salting out." Using the "dry drop test" described above we found there was a considerable increase of birefringence upon adding such salts. X-ray diffraction patterns from samples containing sulfate salts demonstrate the characteristic scattering from amyloid filaments but superimposed on reflections from crystallized salt. Reducing the scattering from microcrystals of sulfate salts will depend on limited rehydration of the sample.

3. Using ultracentrifugation to orient A-beta assemblies. We have explored the method of orientation of elongated particles by centrifugation, which has been successfully applied to tobacco mosaic virus and actin filaments, assemblies that have approximately the same dimensions ($100 \text{ \AA} \times 10,000 \text{ \AA}$) as A-beta fibers. It was previously shown for actin filaments that concentrating by ultrafiltration of solutions containing performed fibrils results in spontaneous orientation of filaments on the filter surface. We used Amicon microconcentrator tubes having a filter cut-off of MW $\approx 3 \text{ kDa}$ and a centrifuge force $\approx 14,000 \text{ g}$ to concentrate our pre-formed fibrillar solutions of A-beta(1-40) (1 mg/ml of protein concentration in PBS solution at pH 7.4). After concentrating solution by factor of ≈ 20 we transferred the gel fraction from the top of the filter into siliconized 0.8-mm thin-walled glass x-ray capillaries and allowed the gel to dry slowly in a 2 T static magnetic field. Preliminary analysis using the polarized light microscope and x-ray diffraction show no indication of orientation in the gel. Electron microscopy will be used to investigate the morphology of the assemblies constituting the gel in an attempt to understand why the orientation failed.

4. Studies on scrapie prion-related peptides help in development of fiber diffraction pattern analysis. Small proteinaceous infectious particles called prions cause certain neurodegenerative diseases in human and animals. Limited proteolysis of infectious scrapie prions PrP^{Sc} yields an N-truncated polypeptide termed $\text{PrP} 27-30$, which encompasses residues 91-231 of PrP^{Sc} and which assembles into 100-200 $\text{\AA}$ -wide amyloid rods. It has been hypothesized that the infectious prion is converted from its non-infectious, cellular form (PrP^{C}) by means of an alpha-helical to beta-sheet conformational change. Secondary structure analysis, computer modeling, and structural biophysics methods support this hypothesis. Residues 90-145 of PrP , which contain the two putative alpha-helical domains H1 and H2, may be of particular relevance to the disease pathogenesis as C-terminal truncation at residue 145 was found in a patient with an inherited prion disease. Moreover, our recent x-ray diffraction analysis (Nguyen *et al.*, 1995; Inouye & Kirschner, 1996a) suggests that the peptide consisting of these residues (designated SHa 90-145) closely models the amyloidogenic, β -sheet core of PrP .

Both for its own intrinsic scientific value and also as an essential aid in the development of analytical tools for interpreting fiber diffraction patterns from amyloidogenic assemblies, we have analyzed in detail the x-ray diffraction patterns of SHa 90-145 (Inouye & Kirschner, 1996b). Two samples were examined: one that was dehydrated under ambient conditions whilst in an external magnetic field (to induce fibril orientation), and another that was sealed after partial drying. The dried, magnetically-oriented sample showed a cross-beta diffraction pattern where the fiber axis (rotation axis) is parallel to the H-bonding direction of the beta-sheets. Electron density projections along the H-bonding and the chain directions were calculated by iterative Fourier synthesis using beta-silk as an initial phase model. The density maps indicated that there were two types of beta sheets, one more electron dense than the other, suggesting that larger and smaller sidechains localized to different beta-sheets. This would arise from folding of the polypeptide in which there are turns in the middle of both the H1 and H2 domains. A monoclinic macro-lattice was found to index all the reflections, including those in the low-angle region. The unit structure of this lattice is likely to be a 40 $\text{\AA}$ -wide beta-crystallite. The partially dried sample showed a sharp, 4.7 $\text{\AA}$ reflection (from H-bonding) and four broad peaks superimposed on monotonically decreasing diffuse scattering. This solution-like scattering was modeled by an anisometric rectangle with a thickness comparable to a single beta-chain. The structure, which occurred during dehydration, could be an intermediate in the alpha-beta transition, suggesting that formation of hydrogen bonding precedes the intersheet interaction and assembly into the amyloid of scrapie prion.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 8/95 EXPIRATION: 8/98

PROJECT IDENTIFICATION: 962-23-08-32

NASA CONTRACT NO.: NAG8-130

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Wiedemeier, H., and Hutchins, M.A. The Temperature-Composition Phase Equilibria in the HgTe-HgI₂ Pseudobinary System. *Z. anorg. allg. Chem.*, vol. 622, 1150-1160 (1996).

Proceedings

Inouye, H., and Kirschner, D.A. "Refined fibril structures: The hydrophobic core in Alzheimer's beta-amyloid and prion as revealed by X-ray diffraction." *The Nature and Origin of Amyloid Fibrils*, CIBA Foundation Symposium No. 199, pp 22-39, John Wiley & Sons, Chichester, United Kingdom and New York, New York (1996).

Presentations

Inouye, H., and Kirschner, D.A. "Intersheet hydrophobic cores in fibrillar amyloid assembled from Alzheimer's disease A-beta and scrapie PrP peptides." 27th annual meeting of the American Society for Neurochemistry, Philadelphia, Pennsylvania, March 1996.

Kirschner, D.A. "Refined Fibril Structures." CIBA Foundation Symposium on "The Nature and Origin of Amyloid Fibrils," Oeiras, Portugal.

Kirschner, D.A. "Amyloid Fibril Structures." CIBA Foundation/Calouste Gulbenkian Foundation, Open Meeting on The Nature and Origin of Amyloid Fibrils, Lisbon, Portugal.

Kirschner, D.A. "Fibrillogenesis in Alzheimer's disease." University of Virginia, April 1996.

Kirschner, D.A. "Trials and tribulations in fabricating oriented amyloid fibrils for x-ray diffraction." Protein Crystal Growth Conference, April 1996, Microgravity Materials Science Conference.

Kirschner, D.A. "Targeting fibrillogenesis in Alzheimer's disease." Pharmaceutical Peptides, Inc., Cambridge, Massachusetts, May 1996.

Applications of Atomic Force Microscopy to Investigate Mechanisms of Protein Crystal Growth

PRINCIPAL INVESTIGATOR: Dr. John H. Konnert

Naval Research Laboratory (NRL)

CO-INVESTIGATORS:

Ward, K.

Naval Research Laboratory (NRL)

Perozzo, M.A.

Naval Research Laboratory (NRL)

Task Objective:

The research objective is to use Atomic Force Microscopy (AFM) to study protein crystal growth mechanisms by extending the pioneering work of Durbin et al (1992) to include crystals other than lysozyme, and by applying image analysis methods not generally available to others to aid in the interpretation of crystal face images observed by this technique. Specific objectives include:

- To modify an AFM liquid sample cell for use as a crystal growth cell for protein crystals. This cell has a flow-through system which will allow protein supersaturation to be controlled by varying the temperature of the crystallization solution bathing the crystal being observed;
- To determine by direct observation of developing crystal faces the mechanism of crystal face growth for a variety of growth conditions including solution composition, degree of protein supersaturation, temperature, growth rate, and microgravity;
- To use crystal etch figures methods and direct observation of growing crystal faces observed by AFM to classify and determine the number of crystal imperfections which occur under a variety of crystal growth rates and conditions, including the examination of faces of single crystals prepared under microgravity conditions;
- To demonstrate that the observed diffraction quality of protein crystals prepared under a variety of conditions can be correlated with the number and type of crystal defects observed using AFM; and,
- To determine whether any observed changes in the appearance of the surface of protein crystals can be correlated with the growth cessation phenomena of protein crystals.

Task Description:

Proteins will be prepared for examination by AFM using conventional vapor diffusion, hanging drop methods, and in the temperature-controlled crystallization cell described by Ward, Perozzo and Zuk (1992).

The goal will be to prepare crystals of a given protein using different growth rates by carefully controlling the degree of supersaturation and other growth parameters. Single crystals prepared for these studies will be characterized by x-ray diffraction analyses using standard data reduction and analysis techniques. The diffraction quality will be quantified using the relative Wilson plot analyses described by DeLucas *et al* (1991).

In addition to preparing crystals under unit gravity conditions, we also intend to submit these proteins for crystallization experiments under microgravity conditions. These experiments will be performed by Keith Ward either as part of the co-investigator protein crystallization program at the University of Alabama-Birmingham or as part of his own Flight Investigation Project which has been submitted in response to the recent NRA.

A number of proteins have been selected for this application of AFM to protein crystal growth studies. Each one is readily available, easily crystallized, and exhibits unique crystallization properties.

Task Significance:

This project will, for the first time, provide unique information about protein crystal growth processes by direct observation of crystal faces in their growth medium. Successful results will provide new evidence for the effect of crystal growth conditions, including microgravity, on the defect structures and diffraction quality of protein crystals.

Results derived from this project will, therefore, be of direct significance to NASA-funded efforts aimed at preparing high-quality protein crystals for structural investigations by effectively utilizing the unique microgravity environment of space platforms.

Progress During FY 1996:

The data collection and processing techniques developed at NRL have been applied to study the growth kinetics of protein crystals in highly supersaturated solutions. The growth of the (110) face of lysozyme crystals under conditions of up to 10 fold supersaturation has been observed. High concentrations of such as these are those under which the majority of the growth occurs for crystals prepared for x-ray diffraction experiments. The data collected with these observations include the rate at which two-dimensional nucleation takes place and the rates at which these nuclei grow.

We have collaborated with Professor Alexander McPherson's group at the University of California at Riverside in the interpretation of the molecular features on the surface of dynamically growing crystals of the protein thaumatin. The details in the AFM data provide direct evidence concerning the number of molecules in the growth unit. The experimental data have been collected in California, and the observed features have been quantitatively modeled with programs developed at NRL with the support of the NASA grant. A paper has been prepared for publication.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 1/93 EXPIRATION: 1/96

PROJECT IDENTIFICATION: 962-23-08-25

NASA CONTRACT No.: H-07973D

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Konnert, J.K. "Atomic Force Microscope Studies of Protein Crystal Growth: (a) Observations at up to 10x Supersaturation, (b) Modeling and Interpretation of Observed Molecular Features." Protein Crystal Growth Conference, Panama City, Florida, April 28-30, 1996.

Regulation of Skeletal Muscle Development and Differentiation In Vitro by Mechanical and Chemical Factors

PRINCIPAL INVESTIGATOR: Dr. William E. Kraus

Duke University Medical Center

CO-INVESTIGATORS:

Truskey, G.A.

Duke University

Task Objective:

This is a biomedical engineering project dealing with the *de novo* growth of three-dimensional skeletal muscle tissue in a culture system. The thrust of the project is the bioengineering of skeletal muscle fibers in culture and involves 1) construction of a device adequate for the study of mature muscle cells in culture and which mimics some of the mechanical responses experienced by skeletal muscle fibers during physical exercise, 2) comparison of biologic maturation of skeletal muscle fibers grown in this device with those grown in the NASA bioreactor, and 3) characterization of the physical and chemical parameters of the culture conditions (e.g., physical stress and strain, metabolite and gas diffusion) that contribute to fiber type alterations in mature muscle fibers.

Task Description:

I. *Investigations of the cell culture conditions that support the development of intact muscle fibers in vitro.* This phase includes construction of and comparison of several devices that will support the growth of mature skeletal muscle fiber bundles in vitro. Preparation for Phase I has required identification of a suitable flexible membrane upon which freshly derived mammalian (rabbit) myoblasts grow and proliferate, identification of a suitable mechanical attachment for the fibers, and identification of stretching parameters that promote muscle fiber alignment. The device has also been designed to support studies of various deforming frequencies on skeletal muscle phenotype. This phase also addresses considerations of the influences of a) extracellular matrix substrate, b) original muscle fiber type from which the cells were derived, c) co-culture of non-muscle cell types in the culture (e.g., fibroblasts, neurons), d) media conditions and e) uniform, gradual physical deformation (mechanical loading) on the ultimate phenotypic characteristics of the resulting fibers. Muscle fiber phenotype is to be determined by using histological staining, immuno-histological staining with fiber type specific antibodies, and the ratio of gene expression for oxidative to glycolytic enzymes. Primary muscle cells will be derived from two sources in the rabbit — the fast-twitch, glycolytic muscle, tibialis anterior and the slow-twitch, oxidative muscle, soleus. Comparisons are to be made between the device designed and built in our laboratory the NASA bioreactor.

II. *Investigations of the mechanical and chemical factors that influence gene expression in developing and maturing skeletal muscle.* Phase II involves investigations of how cellular signaling pathways may be involved in the modulation of skeletal muscle fiber type with changes in loading, activity, metabolic substrate, and hormonal influences. Phase II of the task entails exploration of external mechanical and chemical factors (e.g., deformation magnitude and frequency, media conditions, growth factors, oxygen) and internal signaling molecules (cAMP, Type II adenylyl cyclase and protein kinase C θ [PKC θ], pH) triggered by external factors that may control the phenotype and metabolism of skeletal myocytes. Mature skeletal muscle fibers of a fast-twitch glycolytic fiber type will be subjected to various loading and mechanical deformation protocols. The effects of mechanical forces on skeletal muscle phenotypes will be determined using the parameters outlined in Phase I. Mechanical forces will be measured, and stress-strain relationships derived and correlated with changes in cellular signaling molecules and gene expression for signaling molecules (Type II adenylyl cyclase, PKC θ) and various markers of skeletal muscle fiber type. In like manner, cultured muscle fibers will be subjected to various conditions of oxygen tension, while controlling for mechanical forces, and changes in muscle fiber type will be determined.

Task Significance:

The development and further characterization of the *in vitro* culturing system described in this task and the technologies and techniques for monitoring and modeling the chemical and mechanical influences on skeletal muscle phenotype and function will provide insight into the cellular processes underlying maintenance of skeletal muscle function in normal and low-gravity environments. Progress in describing the cellular signaling pathways involved in transducing mechanical signals generated by changes in activity to alterations in the intracellular milieu, as

described in this proposal, may help provide clues to better countermeasures and therapeutic interventions for maintaining skeletal muscle function during space flight.

Progress During FY 1996:

Substantial progress has been made for both Phases I and II as outlined in the task description.

Phase I

Primary Cell Cultures

Cell culture conditions for the isolation, propagation, and differentiation of myoblasts isolated from adult rabbit fast- and slow-twitch muscle have been characterized. We have defined a set of conditions whereby we can produce a population of healthy myoblasts that can be induced to fuse into multinucleated myotubes. These myotubes spontaneously contract and immunostain for sarcomeric proteins such as α -actinin, myosin, and titin. Electron microscopy demonstrates that the myotubes have well-ordered sarcomeres with localized mitochondria and sarcoplasmic reticulum. A substantial number of aliquots of these cells have been stored frozen for later use.

Stretch Device

Construction of the device used to study mechanical loading of skeletal muscle cells has been completed. We have spent considerable time refining the apparatus in order to optimize cell growth and minimize the risk of contamination. We determined that gas sterilization by ethylene oxide, which is cited in the literature as a method of sterilization of similar devices, is not appropriate. Silastic membrane sterilized in this manner is unable to support the growth of mammalian myoblasts. The design of our apparatus allows us to sterilize the base and motor by gas and separately sterilize the silastic wells by autoclaving. We are now growing C_2C_{12} cells, a murine myoblast cell line, in the device to further optimize conditions. We are currently testing parameters such as cell density and are exploring various attachment matrices. We have begun experiments in which we subject these cells to a stretch pattern that mimics murine long bone growth. We are testing software so we can quantitate morphological alterations in cells exposed to mechanical loading. Parameters to be measured include myotube alignment, length, diameter, and branching. We are also carrying out further studies to characterize the silastic membrane and its responses to stretch. In addition, characterization of cellular morphology by immunohistochemistry and quantification of cellular proteins by Western blotting is under way.

Rotating-Wall Vessel (RWV) - NASA Bioreactor

We have made considerable progress with respect to cell culture in the RWV. As with the stretch device, we are initially carrying out experiments using C_2C_{12} cells to determine appropriate culture conditions. C_2C_{12} cells have been grown in the RWV on cytodex microcarrier beads. In preliminary experiments, we have observed that the myoblasts are able to proliferate and differentiate in this environment. However, when compared to sister cultures grown in static monolayer cultures or grown in a teflon bag as a 3-dimensional static control, the extent of fusion of myotubes is reduced in the RWV. These experiments will be repeated and western blotting will be performed to quantitate amounts of contractile proteins. We have also begun to characterize the forces experienced by the cells in the RWV. Measurements of the motion of the beads in the RWV at different stages of growth, in conjunction with measures of sedimentation velocity and aggregate radius, have allowed us to calculate the average shear stresses on the cells.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 9/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-23-01-18

NASA CONTRACT NO.: NAG9-810

RESPONSIBLE CENTER: JSC

Neuro-endocrine Organoid Assembly in Vitro

PRINCIPAL INVESTIGATOR: Dr. Peter I. Lelkes

University of Wisconsin, Milwaukee

CO-INVESTIGATORS:

Unsworth, B.R.

Marquette University

Task Objective:

The specific aims of our project, entitled "Neuro-endocrine Organoid Assembly *In Vitro*" are as follows:

- 1) To assemble adrenal medullary endothelial and parenchymal cells into functional organoids. Progress will be monitored by evaluating a) morphology (light microscopy and ultrastructure), b) intercellular communication (immunocytochemistry), c) functional maturation and its hormonal control by corticosteroids, and d) the expression of phenotypic, biochemical, and molecular markers.
- 2) To compare the usefulness and efficacy of NASA vessels with conventional co-culture systems (monolayer culture, suspension culture and 3-dimensional gel assembly). The time course and the extent of neuro-endocrine cell differentiation under the different culture conditions will be evaluated (as in 1).

Task Description:

Our long-term research goal is to understand fundamental mechanisms of neuro-endocrine gland assembly and differentiation. In our particular model system, the adrenal medulla, neural crest-derived cells of the sympathoadrenal lineage, differentiate into neuro-endocrine chromaffin cells. We are particularly interested in the role of the microenvironment in this process. We have previously shown that during assembly and maturation of the adrenal medulla, as in other endocrine organs, parenchymal cells and endothelial cells interact through reciprocal, intercellular signals. Such signals may constitute soluble factors or heterotypic cell contacts or may be derived from organ-specific extracellular matrix components. These cues comprise part of the epigenetic repertoire, which induces the ordered differentiation of both cell types into what is known as the "endocrine structure."

Using conventional 2-D culture techniques, we have shown that in co-culture with adrenal medullary endothelial cells, chromaffin-cell-derived pluripotent PC12 cells differentiate towards the neuroendocrine phenotype. We, therefore, hypothesize that capillary endothelial cells in the adrenal medulla provide some of the organ-specific, differentiative cues which contribute to the neuroendocrine differentiation of the chromaffin precursor cells.

In this ground-based project, we extend our ongoing *in vitro* studies on the mechanisms of organ-specific differentiation by using alternate methods of co-culture. We are exploiting the enhanced potential offered by the NASA vessels to analyze the temporal assembly of co-cultured adrenal medullary endothelial and parenchymal cells into functional tissue-like assemblies. Concomitantly, we also investigate the organ-specific assembly and differentiation of rat PC12 pheochromocytoma cells, tumor cell lines derived from chromaffin cells, into functional organoids. The simulated microgravity environment has been shown to randomize gravitational vectors and minimize detrimental shear forces routinely encountered in conventional three-dimensional suspension cultures in spinner flasks. Based on morphological, biochemical, and molecular biological data obtained in our PC12 cell studies, we anticipate that the favorable culture conditions in the NASA vessel will accelerate differentiative, heterotypic cell-cell contacts and thus lead to the assembly of functional adrenal medullary organoids *in vitro*.

Task Significance:

This ground-based study is relevant to NASA's Cell Culture Biotechnology mission from several vantage points.

Programmatically, we attempt in this study to recreate neuro-endocrine organoids *in vitro* by co-culturing different cells isolated from the adrenal medulla. Towards this goal, we are using "simulated microgravity" in the NASA RWV Bioreactors as a novel, alternate approach to conventional suspension culture in spinner flasks. The unique conditions in the NASA vessels are believed to enhance cellular interactions and thus differentially accelerate and/or facilitate these processes. In complementing a number of other parallel studies within this program, our project is the first one specifically designed to examine the effects of microgravity on heterotypic interactions between

parenchymal cells and microvascular endothelial cells isolated from the same organ, namely the rat adrenal medulla. Such intercellular interactions are believed to be of importance during all phases of the development of endocrine organs, from the earliest stages of embryonic genesis through postnatal maturation.

In terms of the scientific goals, we are using ground-based RWV Biotechnology for the recreation of functional neuroendocrine organoids. In the past year(s), we demonstrated that PC12 cells, a well-defined model for neuroendocrine differentiation, were responsive to "simulated microgravity" in the RWV bioreactors. Significantly, our study of neuroendocrine organoid assembly combines structural and functional analyses. Moreover, we have for the first time assessed signal transduction mechanisms which may be affected by the culture conditions in the RWV bioreactors, thus enabling us to search for and to identify microgravity-sensitive genes. Our current and future studies will advance our basic scientific knowledge about cellular and molecular mechanisms governing the assembly and organ-specific differentiation in co-cultures of parenchymal and endothelial cells derived from neuroendocrine tissues. Thus, we have provided evidence that the "simulated microgravity" conditions can be used as a tool to recreate a functional neuroendocrine organoid. Our results further strengthen the notion that the NASA RWV cell culture biotechnology is uniquely suited for the generation of differentiated, functional tissue-like organoids.

In terms of a potential "clinical usefulness" of our studies, neuroendocrine organoids are currently being investigated as replacement and/or transplantation tissues in neurodegenerative diseases and for the management of chronic pain. Thus, we anticipate that NASA RWV cell culture biotechnology will provide the most appropriate cell culture venue to recreate functional, macroscopic organoids which will be useful as replacement tissue in neurodegenerative diseases (e.g., Parkinson's Disease).

The long-term goal, beyond the scope of this proposal, is to provide NASA with a well-defined model for future in-flight testing of the effects microgravity in space on the assembly of functional neuroendocrine organoids.

Progress During FY 1996:

In the past fiscal year, our major focus was to further solidify our findings of organoid assembly and tissue-specific differentiation in PC12 pheochromocytoma cells cultured under simulated microgravity in the NASA Rotating-Wall Vessels (RWVs). Moreover, we continued to evaluate the extent of tissue-like assembly and differentiation in co-cultures of PC12 cells with adrenal medullary endothelial cells (RAMEC).

We further developed quantitative RT-PCR-based assays, which enable us to quantitate the enhancement of neuroendocrine differentiation at the gene level. We found that simulated microgravity culture conditions specifically enhance the expression of phenylethanolamine-N-methyl transferase, the enzyme responsible for the conversion of norepinephrine to epinephrine. By contrast, none of the other catecholamine-synthesizing enzymes such as tyrosine hydroxylase, dopa-decarboxylase, and dopamine- β -hydroxylase were affected by the low shear environment in simulated microgravity. In contrast, in high shear experiments in stirred fermentors, the activities of tyrosine hydroxylase and dopamine- β -hydroxylase were increased.

Significant progress was also achieved in quantitating the effects of simulated microgravity on the expression of extracellular matrix proteins using quantitative RT-PCR. In both PC12 and RAMEC, the culture conditions in the RWV-elevated cells we a unique elevation of collagen type IV under simulated microgravity but not of fibronectin.

Furthermore, we obtained additional evidence for the involvement of tyrosine phosphorylation as a potential mechanism of gravity-sensitive signal transduction. Our recent results confirm that simulated microgravity alters the pattern of tyrosine phosphorylation in PC12 cells exposed to simulated microgravity both for short-term (less than one hours) and for prolonged periods of time (10 days). These findings open the door to a whole new set of experiments aimed at testing the hypothesis that protein phosphorylation-dependent cellular signaling may be the prime candidate for microgravity-sensitive sensing in cultured cells.

We are continuing to make progress in establishing a co-culture system between adrenal medullary endothelial cells and PC12 pheochromocytoma cells. The current focus in this part of our project is to establish quantitative enumeration techniques for accessing the fractional contribution of two different cell types to heterotypic organoid assembly. Our future research will be aimed at evaluating the effects of co-culture conditions on the neuroendocrine expression and the functionality of the ensuing organoids.

Taken together, our findings suggest that simulated microgravity provides a unique environment which enables tissue-specific assembly and neuroendocrine differentiation of PC12 cells towards the adrenergic, chromaffin cell phenotype of the parental cells. Moreover, our data indicate that the pattern of gene activation in this unique cell culture environment differs from that in other three-dimensional culture modalities in which cells are cultured in aggregate/suspension cultures. Future experiments are designed to establish the cellular and molecular basis for these differences.

Based on the results of our *in vitro* studies, we have been invited to participate as guest researchers in an upcoming Mir/Space Shuttle Mission. PC12 cells will be transported aboard STS-84 onto Mir, and the cells will be propagated during prolonged exposure in microgravity. We have designed a set of experiments and analysis to evaluate the effects of this "actual" microgravity scenario on PC12 cell organoid assembly differentiation.

As an offshoot of this project, we have been funded to study, in collaboration with Dr. Timothy Hammond (Tulane University) the effects of simulated microgravity on renal cell organoid assembly and differentiation. Progress in that project is detailed separately.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 11/92 EXPIRATION: 11/95

PROJECT IDENTIFICATION: 962-23-01-12

NASA CONTRACT NO.: NAG9-651

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Lelkes, P.I., Galvan, D.L., Hayman, G.T., Goodwin, T.J., Chatman, D.Y., Cherian, S., Garcia R.M.G., and Unsworth B.R. Simulated microgravity conditions enhance differentiation of cultured PC12 cells towards the neuroendocrine phenotype. *In Vitro Cell and Developmental Biology, Animal*, (Submitted).

Presentations

Galvan, D.L., Hayman, G.T., Goodwin, T.J., Chatman, D.Y., Unsworth, B.R., and Lelkes P.I. "Simulated microgravity induces neuroendocrine differentiation of PC12 pheochromocytoma cells." 1996 World Congress on In Vitro Biology, San Francisco, CA, June 22-27, 1996.

Galvan, D.L., Lelkes, P.I., Wankowski, D.M., Goodwin, T.J., and Unsworth, B.R. "Simulated microgravity conditions enhance neuroendocrine organoid formation in vitro." Aviation and Space Medicine Association, 67th Annual Scientific Meeting, Atlanta, GA, May 5-9, 1996.

Galvan, D.L., Liu, J., Wankowski, D.M., Lelkes, P.I., and Unsworth B.R. "Differential modulation of extracellular matrix protein expression in adrenal medullary cells cultured under simulated microgravity conditions." *Mol. Biol. Cell*, Nov. 6S:975. 1995.

Multidisciplinary Studies of Cells, Tissues, and Mammalian Development in Simulated Microgravity

PRINCIPAL INVESTIGATOR: Prof. Elliot M. Levine

The Wistar Institute

CO-INVESTIGATORS:

Herlyn, M.

The Wistar Institute

Spain, L.

The Wistar Institute

Panettieri, L.

University of Pennsylvania School of Medicine

Litt, M.

University of Pennsylvania

Pollack, S.

University of Pennsylvania

Meaney, D.

University of Pennsylvania

Task Objective:

Our joint research team from The Wistar Institute and the University of Pennsylvania is establishing nine different cell, tissue, and embryonic systems to be cultured in low shear NASA bioreactors which simulate microgravity. Employing these model systems, we will achieve the following objectives:

- a. Develop optimum cell culture conditions for propagation of a number of three-dimensional complex tissues in current NASA bioreactors, and investigate the effects of simulated microgravity on these model systems at the molecular, biomechanical, cellular, and embryonic levels.
- b. Produce advanced bioengineering enhancement of NASA bioreactor technology and set the ground work for future flight proposals by reiterative combination of hands-on experience with theoretical modeling and prediction.

Task Description:

We are employing multiple culture systems to provide an in-depth evaluation of the effects of low shear and simulated microgravity and the general utility of bioreactor technology. Considered at the cellular and molecular levels, the hypothesis inherent in our approach is that biomechanical forces such as gravity and shear stimulate responses from cells, tissues, and embryos. Initial transduction of mechanical forces into cells involves components such as surface and adhesion receptors and signaling mechanisms including protein kinase C and calcium fluxes. These, then, are translated into alterations in cell association, matrix synthesis, proliferation, migration, differentiation, and gene expression. Each of our projects is testing one or more of the components of this hypothesis. As we progress, we will directly compare microgravity effects on various parameters (e.g., calcium fluxes) in our different model systems. The cell and tissue types being studied are vascular endothelial and smooth muscle, embryonic vascular and cardiovascular, breast and skin, airway smooth muscle, bone, and thymus.

Conclusive studies of the effects of simulated microgravity and development of improved bioreactor technology demand a systematic approach. Applying and enhancing this technology requires rigorous characterization of the biomechanical environment of cells, organ systems, or embryos in the bioreactor. Such characterization is necessary for a quantitative understanding of the altered mechanical stimulus/cellular response studies in all of the proposed projects. The output of our bioengineering studies will influence ongoing experimental design and interpretation of data from our other projects which relate gravity-related stress stimuli to the transduction, biochemical, and morphogenetic pathways of cells, organs, and embryos.

Task Significance:

The significance of our studies resides in testing the hypothesis that biomechanical forces, such as gravity and shear, evoke significant responses from cells, tissues, and developing embryos. The nature of the response we discover will be important in evaluating the cellular effects of microgravity. The initial transduction of mechanical forces into cells involves components such as surface and adhesion receptors and signaling mechanisms including protein kinase C and calcium fluxes. These then are translated into alterations in cell association, matrix synthesis, proliferation, migration, differentiation, and gene expression. Each of our projects is testing one or more components of this hypothesis. As we achieve our objectives, we will be able to reach generalized conclusions by directly comparing microgravity effects on, as one example, calcium fluxes in the different model systems.

Our studies will also have practical importance in developing improved cell/tissue culture model systems. Although not always recognized, the usual static or suspension culture conditions also exert significant biomechanical forces (i.e., unidirectional gravity vector and/or high shear) on cells. In such cases, cell growth and differentiation as well as tissue reconstitution are adversely affected. Thus, we anticipate that bioreactor-grown cultures will more closely resemble *in vivo* tissue than cultures grown under ordinary conditions.

Progress During FY 1996:

The progress achieved by the various subprojects during the initial eight-month period since funding began is described below:

Bioengineering Projects: A prototype multiple-HARV unit has been designed and is in testing stage. This unit will allow six disposable-type HARV bioreactors to operate from a single drive assembly in the same incubator space required for a standard HARV unit. A prototype particle visualization and tracking system has been designed and built. The system allows light video tracking and digital recording of particle trajectories in the HARV and is being extended to permit fluorescent particle tracking as well. Software for computer analysis of the trajectories to permit validation of theoretical analysis of particle motions is being developed.

Theoretical calculations of single particle trajectories in the HARV have been carried out giving prediction of particle position with time as a function of system parameters (particle radius, initial position, medium viscosity and density, particle density, reactor dimensions) and rotational speed. The calculation of software and tracking system computer permit on-line calculation and comparison of actual and predicted particle motions. Initial tests indicate that the predicted motions agree with the observations, allowing quantitative estimates of reduced gravity for various conditions in the HARV.

We have identified mechanical stimuli which affect cell growth in the HARV and have initiated cell studies to determine their significance. Studies using primary rat calvaria osteoblasts and 17/2.5 ROS sarcoma cells plated on T25 culture flasks specifically looked at static hydrostatic pressure as well as dynamic rotational pressure. preliminary results from cell growth assays (DNA synthesis and AP production) and visual examination indicate that reduced hydrostatic pressure as well as rotational dynamic pressure (simulated microgravity) significantly alter cell proliferation and morphology in the primary cells but not in the sarcoma cells. Additional studies essential for understanding cell growth and biomechanics under HARV conditions will examine shear forces, convective transport, medium properties, intermittent wall contact, cell attachment to carriers and reactor surfaces, and surface chemical and mechanical interactions with cells.

Vascular and Developmental Morphogenesis Projects: Conditions have been developed for the culture of human vascular endothelial (HVECs) and smooth muscle cells (HVSMTs) in the NASA bioreactor. As "non-rotating controls," we have been using gas-permeable teflon bags. We discovered that adherence of HVECs and HVSMTs is affected by differences (e.g., matrix production) among cell strains. Depending on cell types and conditions, HVECs and HVSMTs can be grown on coated or uncoated beads, polyglycolate scaffolding, and collagen spheres ("Cultispheres"); formation of multicellular aggregates is common. In many cases, viability and proliferation of cultures (as measured by glucose consumption) has been maintained for 2 to 4 weeks or more. Cell densities and culture morphologies are assessed both by phase microscopy and staining with fluorescent dyes such as DAPI and DiI. Differentiated functions are being monitored by immunofluorescent assays for smooth muscle cell actin and endothelial cell factor VIII-related antigen.

The effects of simulated microgravity and NASA bioreactor culture on development of the cardiovascular system is being studied by employing *ex utero* culture of murine embryos. Culture conditions have been optimized and murine embryos have been successfully cultivated under standard and bioreactor conditions. Crucial developmental events occur in murine embryos between 7.5 and 10 g.d., and it is during this time period that we are closely monitoring standard and bioreactor-grown embryos for defective or enhanced cardiovascular development.

Skin and Breast Tissue Morphogenesis Projects: Our objective is to develop culture conditions allowing the reconstruction of skin and breast tissue. Our investigations have begun with construction of a "dermis" made of rat tail collagen type I seeded with fibroblasts isolated from human dermis (5-50x10⁵ cells in 3 ml collagen per 60 mm dish). Under "stressed" conditions, fibroblasts constrict gelled collagen by more than 60% within 4 days, with a maximum at 7 days. More than 70% of viable cells can be recovered 7 days later. After

digestion of collagen, cells continue to proliferate. Under "non-stressed" conditions, the collagen is, after hardening, lifted off the dish, allowing faster constriction (2 days) by fibroblasts. Fourteen days later, cell viability in "non-stressed" cultures is over 95%. Therefore, we conducted our subsequent studies using "non-stressed" conditions. We found no differences in viability of fibroblasts in either stationary cultures or under microgravity conditions. Critical for growth and viability in the NASA bioreactor is the maintenance of optimum pH and oxygen concentration which are monitored daily and adjusted as needed.

The second step in our studies was to co-culture melanocytes and keratinocytes for construction of an epidermis. We initiated cultures under stationary conditions by seeding at a ratio of 5 keratinocytes to 1 melanocyte. Confluent cultures were exposed to air by placing the membrane in the air interface. Under these conditions, cells receive nutrients but start to differentiate by forming multiple layers. We are currently testing the optimal membrane that allows us to culture epidermal sheets in the HARV. Our initial results indicate some problems with membrane curling, thus we are experimenting with different materials which will maintain even cell sheets. We also have initiated combined cultures in which "epidermis" was grown on "dermis." This "skin equivalent" was then placed into the HARV and maintained for up to 10 days. Beginning at day 8, some membrane disintegration was observed. Fixed specimens showed considerable multilayer formation. We currently are repeating experiments to examine the differentiation status of the cells in multiple layers.

In the next few months, we will continue to improve growth conditions for dermis and epidermis. An important goal will be to monitor gene expression in the reconstructs at different stages during microgravity culture and compare these HARV-derived cultures directly with those from stationary cultures. At the same time, we have constructed several adenoviral vectors which will allow us to modulate gene expression in the cells; these include human bFGF, VEGF, PDGF A, PDGF B, pleiotrophin, IL-8, and MCP-1. Within the next year, we expect to determine the biological significance of each growth factor for skin morphogenesis. In year 2, our experiments will be directed towards the reconstruction of human breast tissue.

Airway Smooth Muscle Projects: To date, we have made substantial progress along the following two lines of research:

1. Growth of human airway smooth muscle (HASM) cells in simulated microgravity. We have successfully grown ASM cells in the NASA HARV and characterized cell growth by a total protein assay as well as direct morphologic examination. Since ASM cells are adherent, it was necessary initially to examine whether ASM cells would proliferate on microcarrier beads and, then, to determine the growth characteristics of myocytes on beads in simulated microgravity. ASM cells were cultured in F12 media containing 10% fetal bovine serum and seeded at a density of 2×10^6 cells/125,000 microcarrier beads. Cells were grown either in a HARV or in tissue culture flasks. In order to determine the effects of microcarrier beads alone on ASM cell growth, ASM cells were also maintained in cell culture bags which prevent adherence of cells to plastic surfaces. After 24 hours, the cultures were arrested in F12 media with 5 mg/ml insulin and 5 mg/ml transferrin for 24h and then stimulated with 10% serum. After 48 hours of serum stimulation, total protein assays were performed on the cultures. Total protein content was compared among cells stimulated with FBS and grown in the HARV, culture bags, and tissue flasks and compared with those treated with diluent alone. Total protein content in cells stimulated with FBS in the HARV, in culture bags and in flasks, increased as compared with that obtained from cells maintained in identical vessels but which were treated with diluent alone, 157%, 166%, and 172%. Morphologic analysis of the cells showed no significant changes in cells grown in the HARV as compared with those grown in either the culture bag or tissue flask. Taken together, these data suggest that simulated microgravity may inhibit ASM cell growth induced by serum. Over the next 12 months, we will determine whether simulated microgravity modulates serum-induced increases in ASM cell number as well as determine whether microgravity also modulates the phenotypic expression of smooth muscle-specific proteins.

2. Developing specific assays to characterize the effects of microgravity on the activation state of ASM cells. We propose to examine the effects of microgravity on the agonist-induced calcium mobilization and protein kinase C activation. Since increases in cytosolic calcium in ASM cells are regulated, in part, by IP_3 -induced release of calcium stores, we developed a specific anion-exchange chromatographic assay to measure phosphoinositol (PI) turnover in cells grown in the HARV. In recent experiments, we have determined that 5mM bradykinin induced a 5.5 fold increase in PI turnover as compared with that obtained in cells treated with diluent alone. In the next two months, we will use this assay to characterize the responsiveness of ASM and bone cells to bradykinin grown in

microgravity. In years 3-4, we will directly measure cytosolic calcium mobilization in cells maintained in simulated microgravity since these methods currently are being developed in collaboration with the Bioengineering Projects.

In order to characterize other critical downstream signaling events that regulate ASM cell proliferation, we have also developed an assay to measure phosphatidylinositol 3-kinase (PI 3-kinase) activation. In preliminary studies, inhibition of PI 3-kinase by wortmannin completely abolished EGF- and thrombin-induced ASM cell proliferation. These data suggest that activation of PI 3-kinase is necessary to mediate ASM cell growth stimulated by growth factors. In the next 12 months, we will examine whether simulated microgravity modulates activation of PI 3-kinase induced by contractile agonists and growth factors.

T-cell Development Project: Our goal is to explore the effects of simulated microgravity on thymic development using the rotating bioreactor system. The first step in this analysis is to determine the viability of fetal thymuses in the bioreactor, then to optimize conditions for growth and differentiation.

We have determined that fetal thymuses older than 16 days are viable in the rotating bioreactor for 2 days. We measured a small, likely insignificant reduction in cellularity of bioreactor-cultured thymuses relative to FTOC conditions, but developmental parameters, such as expression of cell surface proteins CD4, CD8, and T-cell receptor were comparable. We conclude, therefore, that the bioreactor *per se* is not detrimental to thymocyte survival.

One very important difference between bioreactor culture (STLV) and standard fetal thymic organ culture (FTOC) is that in bioreactors the thymuses are totally submerged in medium while in FTOC the thymus lobes are exposed at the air/medium interface. Watanabe and coworkers have shown that thymus development can occur in submerged cultures if the partial pressure of oxygen in the medium is between 50 and 70%. Our first step, therefore, was to attempt to maintain O₂ in the bioreactor medium at the desired level. This has been problematic; we have found that O₂ levels are variable and difficult to maintain in the appropriate range. We are now exploring other configurations of bioreactors and more controlled gas delivery to improve the performance of the bioreactors.

Nevertheless, in one experiment, O₂ levels were maintained at comparable levels in the STLV and in the submerged non-rotating cultures (53% versus 66%, respectively). To test the effects of bioreactor culture on proliferation and differentiation, thymuses at 14-15 days of gestation were tested. Thymuses were compared after 5 days of STLV culture, FTOC culture, and submerged non-rotating (SNR) cultures. FTOC- and SNR-cultured thymuses exhibited ovoid or flattened morphology, and the thymocytes proliferated 10-fold over the 5-day culture period, and differentiated as assessed by increased expression of CD4, CD8, and T-cell receptor. In contrast, STLV-cultured thymuses exhibited spheroid morphology, and neither proliferated or differentiated. Although just one experiment, these results suggest that conditions in the rotating bioreactor can have profound effects on T-cell development in the thymus. More experiments are needed to determine whether these effects are reproducible and whether bioreactor microgravity is a determining variable.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 8/95 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 963-45-23-21

NASA CONTRACT NO.: NAG9-832

RESPONSIBLE CENTER: JSC

Analysis of Electrophoretic Transport of Macromolecules using Pulsed Field Gradient NMR

PRINCIPAL INVESTIGATOR: Dr. Bruce R. Locke

Florida State University

CO-INVESTIGATORS:

Moerland, T.S.

Florida State University

Task Objective:

The scientific objective of the present work is to apply pulsed field gradient nuclear magnetic resonance (PFGNMR) spectroscopy to the analysis of electrophoretic and diffusive transport of biological macromolecules in solutions of polymers, in gels and in gel-like media. PFGNMR offers the major advantage of allowing for measurement of the rates of transport of a wide range of molecules in media that is not necessarily optically transparent. A limited amount of work has been reported in the literature to show that PFGNMR can be applied to diffusion and electrophoresis; however, further development and study is necessary to apply the method to transport of larger macromolecules in a wider range of materials.

Task Description:

The goal for the first year of this project is to use PFGNMR, which is a well established method for measuring diffusion coefficients, to measure diffusivity of small molecules in gels and in gel-like media. In addition, small probe compounds will be used to investigate structural aspects of the polymer solutions, the gels, and gel-like media through measurement of the hindered diffusion in such media.

Task Significance:

The production of biological macromolecules for medical, consumer, and industrial applications is often limited by the degree of purity to which these compounds can be manufactured. Electrophoresis is a purification technique that utilizes an applied electrical field to separate macromolecules on the basis of the charge and size of the macromolecule. Electrophoresis is performed in solutions of polymers or gels and microgravity conditions. The studies in the present work involve the use of pulsed field gradient nuclear magnetic resonance (PFGNMR) to study the motion of biological macromolecules in gels and solutions in order to improve our understanding of how these molecules can be separated by electrical fields.

Progress During FY 1996:

During the first year of this project studies of the self diffusion of water in acrylamide gels of various concentrations has been performed in order to assess the technique and to determine structural features of these gels. An extensive set of experiments on water self-diffusion in polyacrylamide gels with various amounts of cross-linker and total monomer was performed using the 600 MHz PFGNMR at the National High Magnetic Field Laboratory. These experiments showed the surprising result that the amount of crosslinking agent did not affect the water self-diffusion. Previous work has been reported on the effects of total monomer on water self-diffusion, however no previous work has reported the effects of the amount of cross-linking agent. In addition, a number of experiments to measure T1 relaxation in the gels to assess structural features has been performed and data analysis of these results is being performed. Work is continuing on the measurement of the effect of cross-linking agent on the self-diffusion of larger probes. The electrophoresis probe for the NMR has been designed and constructed, and it is now being installed and tested on the 600 MHz NMR.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 1
PhD Students: 0

TASK INITIATION: 8/95 EXPIRATION: 8/96

PROJECT IDENTIFICATION: 962-24-08-18

NASA CONTRACT NO.: NAG8-116

RESPONSIBLE CENTER: MSFC

Ground-Based Program for the Physical Analysis of Macromolecular Crystal Growth

PRINCIPAL INVESTIGATOR: Dr. Alexander J. Malkin

University of California, Riverside

CO-INVESTIGATORS:

McPherson, A.
Kuznetsov, Y.G.
DeYoreo, J.J.
Land, T.

University of California, Riverside (UCR)
University of California, Riverside (UCR)
Lawrence Livermore National Laboratory (LLNL)
Lawrence Livermore National Laboratory (LLNL)

Task Objective:

The general objective of this research is to gain a better understanding of the physics of macromolecular crystallization. These include development and application of the *in situ* high resolution techniques for both studies of the growth phenomena and mass transport in protein and virus crystal growth.

Task Description:

To achieve the objectives of this investigation, we are applying a combination of physical *in situ* techniques such as atomic force microscopy, conventional Michelson and phase shift Mach-Zehnder interferometry and inelastic light scattering for the quantitative investigation of the nucleation and crystallization phenomena for different proteins and viruses. The specific aims of this investigation are:

- determination of the sources of step generation for different macromolecular systems
- investigations of the surface morphology and kinetics of macromolecular crystallization
- determination of the fundamental kinetic and thermodynamic parameters, which govern macromolecular crystallization
- studies of the defect structure and mechanisms of impurity action
- investigation of the relative importance of transport processes versus surface kinetics
- determination of the concentration gradients around growing and dissolving crystals

Task Significance:

Macromolecular crystallization currently is highly problematic, to such an extent that it has become the rate limiting step to the broader application of x-ray diffraction analyses in molecular biology and biochemistry, which in turn has significant adverse effects on the progress of biotechnology in general. This is true, in a large part, because little is known of the physics of macromolecular crystallization. Crystallization experiments in space provide a significant improvement in crystal quality for a number of protein and virus crystals. In order to evaluate the impact of microgravity in macromolecular crystallization, it is necessary to compare the physics of crystallization in both environments. Increased understanding of the mechanisms of macromolecular crystallization might be expected to result in the development of new growth techniques and contribute to the medical and pharmaceutical applications of biological macromolecules.

Progress During FY 1996:

During the past year we have focused on application of *in situ* atomic force microscopy (AFM) for studies of the growth mechanisms and kinetics of crystallization for different protein and virus systems. These included canavalin, thaumatin, apoferritin, catalase, lysozyme and satellite tobacco mosaic virus (STMV).

This investigation demonstrated that most of the crystals grew on steps generated either by two dimensional nuclei or screw dislocations. The dominant growth mechanism for cubic STMV crystals at moderate to high supersaturation was growth by addition of three dimensional nuclei. Adsorption of three dimensional nuclei were also commonly observed on the surfaces of growing thaumatin, canavalin, catalase and lysozyme crystals as well. This resulted in the appearance of the multilayer stacks, which grew tangentially and in the normal direction due to two dimensional nucleation on the top. Thickness of these three dimensional nuclei varied from no more than 2 to more than 10 layers. Surfaces of apoferritin crystals were atomically rough and grew by a rarely encountered mechanism, normal growth, usually associated with melt or vapor phase crystallization. Thus those

macromolecular systems investigated so far crystallize by all of the classical growth mechanisms known for conventional crystals.

Strong directional kinetic anisotropy in the tangential step growth rates in different directions was observed in thaumatin crystallization. From the supersaturation dependence of tangential step rates, the kinetic coefficient of the steps $b_{\langle 011 \rangle}$ was determined to be 2×10^{-4} cm/sec. The supersaturation dependence of the rate of two dimensional nucleation was measured, and this yielded the supersaturation dependence of the normal growth rate. From these data the surface free energy of the step edge was calculated to be a $\Delta 0.4$ erg/cm² for $s > 0.8$, and 0.2 erg/cm² for $s < 0.8$. It was suggested that at $s < 0.8$, two dimensional nucleation was not homogeneous and occurred at sites more active than normal (e.g., at defects or sites of impurity incorporation). Values of a in the range of $0.4 - 0.7$ erg/cm² were also obtained based on the sizes of critical nuclei, both for growth on dislocations and for growth by two dimensional nucleation.

Similar values for the kinetic coefficient and surface energy of the step edge were found for the crystallization of canavalin and STMV as well. These parameters are two-three orders of magnitude lower than for inorganic crystals grown from solution.

Sedimentation and incorporation of microcrystals and debris particles were observed. Incorporation of microcrystals and foreign particles typically resulted in the formation of defects. Examples of several of the different classes of defects that occur in protein and virus crystals were visualized. These ranged from point (vacancies) to linear (dislocations) and planar (stacking faults) defects. In addition, the defect density in several different macromolecular crystals was calculated and found to be several orders of magnitude greater than is commonly found in conventional crystals.

In situ phase shift Mach-Zehnder was utilized to study concentration gradients around growing crystals. Depletion zones were observed around growing lysozyme and STMV crystals.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/95 EXPIRATION: 7/99

PROJECT IDENTIFICATION: 962-23-08-46

NASA CONTRACT NO.: NAG8-116

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Land, T.A., Malkin, A.J., Kuznetsov, Yu.-G., McPherson, A., and DeYoreo, J.J. Mechanisms of protein crystal growth: An atomic force microscopy study of canavalin crystallization. *Physical Review Letters*, vol. 75, no. 14, 2774-2777 (1995).

Malkin, A.J., Kuznetsov, Yu.-G., and McPherson, A. Incorporation of microcrystals by growing protein and virus crystals. *Proteins: Structure, Function and Genetics*, vol. 24, 247-252 (1996).

Malkin, A.J., Kuznetsov, Yu.-G., Glantz, W., and McPherson, A. Atomic force microscopy studies of surface morphology and growth kinetics in thaumatin crystallization. *J. Physical Chemistry*, vol. 100, 11736-11743 (1996).

Malkin, A.J., Kuznetsov, Yu.-G., Land, T.A., DeYoreo, J.J., and McPherson, A. Mechanisms of growth for protein and virus crystals. *Nature Structural Biology*, vol. 2, no. 11, 956-959 (1995).

Malkin, A.J., Land, T.A., Kuznetsov, Yu.-G., McPherson, A., and DeYoreo, J.J. Investigation of virus crystal growth by *in situ* atomic force microscopy. *Physical Review Letters*, vol. 75, no. 14, 2778-2881 (1995).

Proceedings

Kuznetsov, Yu.-G., Malkin, A.J., and McPherson, A. "Interferometric studies of macromolecular crystal growth." *Proceedings of the 6th International conference on crystallization of biological molecules*, 58 (1995).

Kuznetsov, Yu.-G., Malkin, A.J., and McPherson, A. "Defect structure of protein and virus crystals studied by *in situ* atomic force microscopy." *Proceedings of the 10th American conference on crystal growth*, 37 (1996).

Land, T.A., DeYoreo, J.J., Malkin, A.J., Kuznetsov, Yu.-G., McPherson, A., and Lee, J.D. "An in situ atomic force microscopy study of canavalin crystal growth." Proceedings of the 10th American conference on crystal growth, 12 (1996).

Land, T.A., Malkin, A.J., Kuznetsov, Yu.-G., DeYoreo, J.J., and McPherson, A. "Investigation of canavalin crystallization using in situ atomic force microscopy." Proceedings of the 6th International conference on crystallization of biological molecules, 77 (1996).

Malkin, A.J., Kuznetsov, Yu.-G., Glantz, W., and McPherson, A. "Atomic force microscopy studies of surface morphology and growth kinetics in thaumatin crystallization." Proceedings of the 10th American conference on crystal growth, 34 (1996).

Malkin, A.J., Kuznetsov, Yu.-G., Land, T.A., DeYoreo, J.J., and McPherson, A. "In situ atomic force microscopy studies of protein and virus crystal growth." Proceedings of the 6th International conference on crystallization of biological molecules, 27 (1995).

McPherson, A., Malkin, A.J., Kuznetsov, Yu.-G., and Koszelak, S. "Incorporation of impurities into macromolecular crystals." Proceedings of the 6th International conference on crystallization of biological molecules, 108 (1995).

Presentations

DeYoreo, J.J., Land, T.A., Malkin, A.J., Kuznetsov, Yu.-G., Lee, J.D., and McPherson, A. "In situ AFM investigation of step dynamics and surface morphological evolution during growth from solutions." Dynamics of Crystal Surfaces and Interfaces, Traverse City, Michigan, August 1996.

DeYoreo, J.J., Malkin, A.J., Land, T.A., Kuznetsov, Yu.-G., Lee, J.D., and McPherson, A. "An AFM study of growth mechanisms and morphologies of solution based crystals." TMS annual meeting, Anaheim, California, February 1996.

Land, T.A., DeYoreo, J.J., Malkin, A.J., Kuznetsov, Yu.-G., McPherson, A., and Lee, J.D. "An in situ atomic force microscopy study of canavalin crystal growth." Protein Crystal Growth, Panama City, Florida, April 1996.

Malkin, A.J., Kuznetsov, Yu.-G., and McPherson, A. "Atomic force microscopy studies of macromolecular crystal growth." East Coast Conference on crystal growth, Atlantic City, New Jersey, October 1995.

Malkin, A.J., Kuznetsov, Yu.-G., Glantz, W., and McPherson, A. "An in situ atomic force microscopy study of thaumatin crystal growth." Protein Crystal Growth, Panama City, Florida, April 1996.

McPherson, A., Malkin, A.J., and Kuznetsov, Yu.-G. "Defect structure of macromolecular crystals." Protein Crystal Growth, Panama City, Florida, April 1996.

Thyroid Follicle Formation in Microgravity: Three-Dimensional Organoid Construction in a Low-Shear Environment

PRINCIPAL INVESTIGATOR: Andreas Martin, M.D.

Mount Sinai School of Medicine

CO-INVESTIGATORS:

Davies, T.F.

Mount Sinai Medical Center

Task Objective:

The objective of this project is to construct, from single thyroid epithelial cells, human thyroid neo-organs (organoids) which will greatly facilitate disease-oriented biological investigations.

Task Description:

This project is a logical extension of our previous work on the generation of thyroid organoids *in vivo*. We have recently demonstrated the spontaneous formation of functional human thyroid organoids in basement membrane matrices transplanted into severe combined immunodeficiency (*scid*) mice. Such organoids show functional, active follicles with normal architecture. They respond to recombinant human TSH with thyroglobulin secretion more than 3 months after organoid construction. Such thyroid organoids allow the extensive and prolonged interaction between thyroid cells and lymphocytes. We expect this model to be an important asset to our ongoing studies of human thyroid autoimmune disease.

We are planning to use the favorable, low-shear environment of the NASA-developed bioreactor to generate high-density follicle thyroid organoids. Such organoids would more closely mimic the thyroid tissue and at the same time retain the advantages of a highly reductionist model in which the organ can be constructed from its separate elements. Improved lymphocyte survival in high density thyroid follicle organoids will be the consequence of increased cell/cell contact, improved antigen presentation, and augmented cytokine concentrations with shortened diffusion distances.

Growth of the resulting cellular (follicular) structures will be conveniently monitored, either by trypan blue exclusion at fixed time intervals during cell culture or by following their entrapment by undiluted basement membrane matrix at the end of culture. Their functional characteristics will be easily assessed using established routine assays, and the use of recombinant TSH will allow biological probing of the structures with a highly defined bio-molecule.

Task Significance:

A reductionist model — one in which a human thyroid organoid can be constructed from its separate elements — will allow disease-oriented biological investigations (e.g., the study of disease-relevant lymphocytes in the human autoimmune thyroid diseases or growth patterns of malignant thyroid tumors).

Progress During FY 1996:

Over the first year of funding, we have made significant progress in establishing the cell culture conditions for human thyroid cells (A. Martin et al., manuscript in preparation). In our previous progress report, we had described the use of the SV40-transformed human thyroid cell line TAD2 in a high-aspect ratio vessel (HARV) that resulted in follicle-like structures. We have now applied our experience with this line to the rotary cell culture of non-transformed human thyroid cells. Using thyroid cells of non-neoplastic origin, we have generated newly formed cell structures that display features of human thyroid tissue — thyroid follicles of perfectly round shape and polarized cells with numerous microvilli (correctly) expressed on the luminal side. In addition to structural studies, we have also demonstrated continued viability of human thyroid cells under rotary cell culture conditions with human thyroglobulin levels greater than 3000 ng/mL. These data demonstrate the feasibility of the rotary cell culture approach to human thyroid tissue engineering and form the basis for future human thyroid tissue-lymphocyte studies.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/95 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 962-23-01-17

NASA CONTRACT No.: NAS9-816

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Martin, A., Matsuoka, N., Concepcion, E., and Davies T. F. Endogenous antigen presentation by autoantigen-transfected Epstein-Barr Virus lymphoblastoid cells: T-cell receptor N-region hydrophobicity relates to thyroid antigen recognition. *Autoimmunity*, 21:223-230 (1995).

Nakashima, M., Martin, A., and Davies T.F. Intrathyroidal T-cell accumulation in Graves' disease: delineation of mechanisms based on in situ T-cell receptor analysis. *Journal of Clinical Endocrinology and Metabolism*, 81:3346-3335 (1996).

Presentations

Martin, A. "Preservation of human thyroid organoids in the scid mouse." International symposium on endocrine cell transplantation and genetic engineering, Giessen, Germany, June 16-19, 1996 (Official satellite meeting of the 10th International Congress of the Endocrinology, Invited Presentation).

Martin, A., Zhang, J., Unger, P., and Shultz L. D. "T-cell-receptor V gene selection in human thyroid organoids." *Thyroid* 5 (Supplement 1): 392, 11th International Thyroid Congress, Toronto, Canada, September 10-15, 1995.

Martin, A., Zhou, A., Unger, P., Katz, N., Gordon, R., and Davies T.F. "Thyroid cell growth under low-shear conditions: Three-dimensional organization of SV40 transformed thyroid cells." 10th International Congress of Endocrinology, June 12-15, 1996.

Nakashima, M. and Martin, A. "Clonal T-cell response to hTSHR-peptide revealed by radio-labelled PCR." *Thyroid* 5 (Supplement 1): 41, 11th International Thyroid Congress, Toronto, Canada, September 10-15, 1995.

Biological Particle Separation in Low Gravity

PRINCIPAL INVESTIGATOR: Dr. D. J. Morré

Purdue University

CO-INVESTIGATORS:

Van Alstine, J.M.

University of Alabama at Huntsville (UAH)

Morré, D.M.

Purdue University

Task Objective:

Subcellular particles play key roles in normal health, as well as the course and treatment of a variety of diseases. Most subcellular particles are not homogeneous but exist in distinct subpopulations with specific functional characteristics. Functional heterogeneity is especially evident in cellular endosomes. Research on such subpopulations is currently limited by a paucity of effective separation methods. Those commonly used (e.g., Phase Partition and Free-Flow Electrophoresis) have both been shown to benefit from low gravity. The objective of this research is to prepare to test the hypothesis that "the low gravity environment of space will allow unparalleled separations of subcellular particles," resulting in enhanced knowledge concerning endosomal subpopulations.

Task Description:

The ground-based research necessary to responsibly evaluate this promising hypothesis and, possibly, test it in low gravity is being undertaken by Purdue University in conjunction with the University of Alabama in Huntsville (UAH). Purdue has expertise on subcellular particle separation by Free-Flow Electrophoresis (FFE) and Phase Partition (PP). UAH has expertise related to flight experimentation involving FFE and PP, as well as the use of polymer coatings and polymer-linked affinity ligands to enhance separations obtained by these methods.

Task Significance:

Physicians and scientists are now in need of a better understanding of what subpopulations of particles exist in cells, how they might contribute to disease, and how they point to new methods to treat disease. Our research is aimed at providing the ability to use space to satisfy this need. The research goal is similar to that for protein crystal growth experiments. Much of the value obtained from protein crystals grown in space is related to new knowledge of the protein structure. So, too, the immediate value in being able to isolate defined endosomal subpopulations will be in the knowledge of their existence and how this enhances current medical hypotheses and treatments. Secondary value will come from obtaining even small samples of purer materials as they may allow us to develop or improve methods for their large scale isolation on earth.

Progress During FY 1996:

1. Development of rapid, nondestructive, method to electrokinetically quantify chemical and polymer groups on native and modified biotechnical apparatus surfaces.
2. Developed enhanced biocompatible polymeric coatings for use in partition and FFE separation methodologies.
3. Refined theory of operation of PEG-affinity derivatives used to enhance both FFE and PP separations.
4. Above theory expanded to include direct comparison to polymer "coated" colloids and flat surfaces.
5. Methodology for endosome isolation and characterization.
6. Isolation and characterization of rat muscle endosomes carrying glucose transporters as a potentially useful ground-based model.
7. Detergent-everted plasma membrane vesicles as endosome models.
8. Work on verification of a relationship between mock gravitational (i.e., centripetal) force effects and the efficiency of the separation processes under study as evidenced by publications and presentations listed.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 8/95 EXPIRATION: 8/96
PROJECT IDENTIFICATION: 962-24-08-17
NASA CONTRACT NO.: NAG8-114
RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

- Malmsten, M., and Van Alstine, J.M. Adsorption of poly(ethylene glycol) amphiphiles to form coatings which inhibit protein adsorption. *J. Colloid Interf. Sci.*, vol. 177, 502-512 (1996).
- Malmsten, M., and Van Alstine, J.M. Adsorption of poly(ethylene glycol) amphiphiles to form coatings which inhibit protein adsorption. *J. Interf. Sci.*, vol. 177, 502-512 (1996).
- Malmsten, M., Lassen, B., Van Alstine, J.M., and Nilsson, U. Adsorption of serum complement proteins C1g and C3. *J. Colloid Interf. Sci.*, vol. 178, 123-134 (1996).
- Morré, D.J., Chueh, P.-J., Wu, L.-Y., and Morré, D.M. The antitumor sulfonylurea-inhibited NADH oxidase activity of HeLa plasma membrane vesicles has characteristics of a protein disulfide-thiol interchange protein. *Mol. Biol. Cell*, vol. 6, no. 328a, (1995).
- Morré, D.J., Wilkinson, F.E., Kim, C., Cho, N., Lawrence, J., Morré, D.M., and McClure, D. Antitumor sulfonylurea-inhibited NADH oxidase of cultured HeLa cells shed into media. *Biochim. Biophys. Acta*, vol. 1280, 197-206 (1996).
- Morré, D.M., Sammons, D.W., Yim, J., Bruno, M., Snyder, T., Reust, T., Mainau, L., Garvey, W.T., and Morré, D.J. Isolation by preparative free-flow electrophoresis and aqueous two-phase partition from rat adipocytes of an insulin-responsive small vesicle fraction with glucose transport activity. *J. Chromatog.*, vol. 680, 201-212 (1996).
- Moya-Camarena, S., Morré, D.J., and Morré, D.M. Isolation and characterization of Golgi apparatus from transformed cell lines in culture. *Mol. Biol. Cell*, vol. 6, no. 328a, (1995).
- Osterberg, E., Bergstrom, K., Holmberg, K., Schuman, T.P., Riggs, J.A., Burns, N.L., Van Alstine, J.M., and Harris, J.M. Protein rejecting ability of surface bound dextran in end-on and side-on configurations. *J. Biomed. Materials Res.*, vol. 29, 741-747 (1995).
- Van Alstine, J.M., Malmsten, M., and Brooks, D.E. Poly(ethylene glycol) amphiphile adsorption and liposome partition. *J. Chromatog.*, vol. 680, 145-155 (1996).
- Van Alstine, J.M., Veide, A., and Tjerneld, F. Phase partition and biotechnology. *Trends Biotech.*, vol. 16, 1-3 (1996).

Proceedings

- Emoto, K., Harris, J.M., and Van Alstine, J.M. "Electrokinetic evaluation of polymer coatings for use in capillary electrophoresis." Electrophoresis Society Meeting, Atlanta, Georgia, May 1996.
- Emoto, K., Harris, J.M., and Van Alstine, J.M. "Improved polymer coatings for use in separation science." 18th International Symposium on Capillary Chromatography Riva Del Garda, Italy, May 20-24, 1996.
- Van Alstine, J.M., and Malmsten, M. "Poly(ethylene glycol) amphiphiles." Industrial Symposium on Surface Chemistry: Wetting and Flocculation, Oslo, Norway, November 8-9, 1995.

Presentations

- Morré, D.J. "tNOX, a new cell surface anticancer drug target (invited presentation)." NASA/NIH. Structure-Based Design Conference. Panama City Beach, Florida, April 25-28, 1996.
- Van Alstine, J.M. "Phase partitioning on earth and in space." Department of Biochemistry, University of Lund, Sweden, Spring 1995.
- Van Alstine, J.M. "Polymer coated surfaces and proteins (invited presentation)." Immunex Corporation, Seattle, Washington, October 26, 1995.

Van Alstine, J.M. "Polymer coated surfaces for improved biosensors (invited presentation)." Pharmacia Biosensor, Uppsala, Sweden, November 9, 1995.

Van Alstine, J.M. "Polymer coatings of significance in low gravity bioprocessing (invited presentation)." NASA/MSFC Space Science Lab, Huntsville, Alabama, January 10, 1996.

Van Alstine, J.M. "Polymer coatings and improved biochemical analyses (invited presentation)." Astra Hässle, Göteborg, Sweden, February 22, 1996.

Van Alstine, J.M.. "Polymer coated surfaces of pharmaceutical significance (invited presentation)." Nycomed AS, Oslo, Norway, February 29, 1996.

Continuous, Noninvasive Monitoring of Rotating Wall Vessels and Application to the Study of Prostate Cancer

PRINCIPAL INVESTIGATOR: Prof. David W. Murhammer

University of Iowa

CO-INVESTIGATORS:

Arnold, M.A.
Cohen, M.B.University of Iowa
University of Iowa

Task Objective:

The primary hypotheses that will be tested in this research are: (1) NIR spectroscopy can be used for the real-time, non-invasive monitoring of glucose, glutamine, lactate, and ammonia in a rotating-wall vessel (RWV), (2) the dissolved oxygen concentration within the RWV can be continuously monitored with an optical oxygen sensor using a radioluminescent light source, and (3) cellular adhesion molecule (CAM) expression by prostate cancer cell lines under microgravity conditions better simulate in vivo conditions than routine tissue culture. The specific objectives that will be undertaken to test these hypotheses are: (1) develop calibration models for glucose, glutamine, ammonia, and lactate in increasingly complex mixtures of components found in prostate cancer cell culture medium, (2) develop and test an optical oxygen sensor with a radioluminescent light source, (3) develop on-line systems for monitoring glucose, glutamine, lactate, ammonia, and dissolved oxygen concentrations in cell cultures grown in RWVs and (4) simulate in vivo prostate cancer expression of CAMs by growing prostate cancer cells in RWVs.

Task Description:

The first phase of this research will involve the development of calibration models for the off-line determination of glucose, glutamine, lactate, and ammonia concentrations in prostate cancer cell medium from a single near-infrared (NIR) spectrum. We will begin with a simple matrix and then systematically evaluate more complex matrices, allowing for potential interferences to be identified and for the development of rational procedures to eliminate the adverse effects of these interferences. In the second phase of this research, methodologies will be developed to interface the NIR spectrometer with a perfusion RWV such that the glucose, glutamine, lactate, and ammonia concentrations within the vessel can be non-invasively monitored. This will involve the use of a bifurcated fiber optic probe to deliver NIR light to the bioreactor contents and to collect reflected spectra for analysis. In addition, this phase of the proposed research will utilize luminescence quenching and indicator absorption spectroscopy to non-invasively monitor the dissolved oxygen concentration and pH, respectively. The information obtained through this monitoring system will be utilized to control the pH and nutrient concentrations within the RWV so that the behavior of prostate cancer cell lines can be investigated under conditions closely resembling those found in vivo. Specifically, the expression of CAMs, which are important for invasion and metastases of this and many other types of cancer, will be evaluated.

Task Significance:

Successful development of non-invasive NIR spectroscopic sensors to monitor critical analytes used in conjunction with non-invasive pH and dissolved oxygen monitoring will clearly revolutionize the operation of bioreactors in general and RWVs in particular. We propose to focus attention on selective monitors for glucose, glutamine, ammonia, lactate, pH, and dissolved oxygen because these are the most critical factors in animal cell cultures and affect the overall production efficiency (quality and quantity) of bioreactors in general. Although our work centers around development of monitors specific for prostate cancer cell lines operated in the perfusion mode, it is important to note that the analytical methods developed here will be applicable to nearly all fermentation processes with minor modifications. Successful completion of this work is expected to have a major impact in the general field of biotechnology because the availability of continuous monitors will enable the development of active feedback control strategies which will dramatically improve production efficiency of nearly all recombinant products. In addition, such NIR monitors will be valuable basic research tools capable of providing chemical information that can be used to study the complex biological reactions associated with recombinant processes. Overall, the proposed NIR spectroscopic monitors will be an enabling technology with many applications

throughout the field of biotechnology. This technology will also greatly benefit future microgravity research since it can be applied to continuously monitor and control bioreactors operating in space.

In addition to the wide ranging benefits resulting from the non-invasive monitoring technology, this research will also address questions regarding the mechanisms involved in invasion and metastasis of prostate cancer. This research phase will greatly benefit from the non-invasive monitoring technology by allowing more accurate simulation of in vivo conditions resulting from environmental control. It is anticipated that the knowledge obtained from these studies will allow for a better understanding of the biology of prostate cancer.

Progress During FY 1996:

A new Nicolet Magna 550 spectrometer was purchased for this project. This spectrometer is equipped with the highest caliber optical components for the NIR spectral range. These components are needed to provide sufficient quality for bioreactor measurements. A series of experiments were performed in order to verify the utility of this spectrometer by measuring overall spectrometer stability, spectral noise levels, and optical throughput. Our detailed comparison revealed that the Nicolet Magna 500 spectrometer is superior to other commercially available spectrometers. Performance of the new spectrometer was further evaluated by comparing the quality of calibration models for glucose from spectra collected with our new spectrometer to that from spectra collected with our modified 740 spectrometer. Results from this initial experiment demonstrated that data collected from our new Magna 550 spectrometer were essentially equivalent to those obtained with our modified instrument. Equivalent performance is indicated by essentially the same level of prediction error for calibration models built from spectra collected with each instrument. The significance of this finding is two-fold. First, the prediction errors are well below the minimum required for accurate bioreactor monitoring. Second, results from our earlier experiments with data collected on our modified spectrometer can be extrapolated with confidence to our new set of experiments with the new instruments, thereby eliminating the need to repeat most of our previous work.

Initial efforts to build and evaluate NIR calibration models for bioreactor monitoring focused on measurements of glucose and glutamine. For these models, NIR spectra were collected with our modified Nicolet 740 spectrometer. Samples were collected during a normal bioreactor run involving a typical insect cell line (Sf-9 insect cells) with the commercially available and commonly used Sf-900 II serum-free growth medium. These bioreactor conditions were selected because we have considerable experience and expertise with this specific system, which simplified the experiment. The bioreactor was run for several days and 20 mL samples were collected periodically. At the end of the run, the spent growth medium was collected and analyzed for glucose and glutamine levels. Standard solutions were then prepared in the spent medium by adding known amounts of solid, dried glucose and/or glutamine. The concentrations of glucose and glutamine for each sample corresponded to the sum of the amount remaining in the spent medium and the amount added. NIR spectra were collected in triplicate for each of the resulting 50 solutions. Calibration models were generated with spectra collected from these standard solutions prepared in spent medium. In addition, twenty four cell-free samples were collected during the bioreactor run, and these samples were analyzed for glucose and glutamine by using standard methods (YSI analyzer for glucose and HPLC with an OPA derivitization method for glutamine). The ability of the resulting calibration models to accurately predict glucose and glutamine levels was assessed by comparing concentrations from these models to those measured by the standard methods. The resulting standard error of prediction (SEP) and mean percent error of prediction (MPEP) were 1.41 mM and 2.3% for glucose and 0.51 mM and 5.2% for glutamine, which are within acceptable tolerances for bioreactor monitoring. More importantly from a method development standpoint, these results demonstrate the ability to accurately quantify glucose and glutamine in media as complex as insect cell growth media. This is particularly noteworthy considering the chemical composition of the calibration matrix (i.e., spent growth medium) is significantly different than that for the samples.

A second bioreactor experiment has been completed where samples were again collected during Sf-9 cell cultivation in a proprietary medium provided by American Cyanamid. This time, NIR spectra of samples were collected with our new Nicolet Magna 550 spectrometer. First, the glucose and glutamine concentrations were measured by standard off-line methods. The spent medium was divided into 25 aliquots which were spiked with random, known amounts of glucose and glutamine. Glucose and glutamine calibration models based on a glucose-glutamine in a buffer study was used to predict the concentrations in the above spent medium samples. Standard errors of prediction of 1.06 and 0.47 mM were found for glucose and glutamine, respectively. Similar studies were conducted with fresh medium. This medium was divided into 25 aliquots which were spiked with random, known amounts of glucose and glutamine. Again, the glucose-glutamine in buffer study was used as a calibration data set. Glucose and glutamine studies resulted in standard errors of prediction of 1.11 and 0.63 mM, respectively. The spent media

samples have also been used as a calibration data set to measure glucose and glutamine in the fresh media samples. These studies resulted in SEPs of 0.53 and 1.06 mM for glucose and glutamine, respectively, with good correlations in the concentrations. Additionally, calibration models have been developed using a portion of three studies — glucose and glutamine in a buffer, in spent media, and in fresh media. Such models were used to predict glucose and glutamine in a subset of samples excluded from the calibration set. These studies resulted in SEPs of 0.52 and 0.34 mM for glucose and glutamine, respectively.

Optical sensors for continuously measuring *in situ* levels of ammonia and oxygen are also under development. Our efforts with sensors for ammonia have focused on the development of a solid-state indicator layer with sufficient sensitivity and accuracy to measure ammonia-nitrogen levels in growth media from bioreactors. After screening a number of potential indicator dyes, we have selected bromocresol blue. Sensors constructed with this indicator possess rapid response times, reversible responses, sub-millimolar sensitivity, and long operational lifetimes. A second generation redoluminescence-powered oxygen sensor is currently being developed and characterized. This device is being designed specifically for implementation within the Engineering Development Unit 1 (EDU-1) flight unit for the RWV reactors. This prototype will accommodate a flowing stream of the perfusion medium and will be sensitive to oxygen levels from 9-180 mm Hg and with an accuracy of ± 5 mm Hg. Our data demonstrate that this sensor has excellent reproducibility and calibration stability.

We have also made progress in characterizing the prostate cancer cells that will be used in future RWV experiments. First, a serum-free medium has been established in our laboratory and several of the cell lines have been grown for numerous passages in this medium. Second, we have been able to grow PC-3 cells both freely in suspension and on microcarrier beads in the RWV. Further work, however, is needed to optimize growth under these conditions. Third, the PC-3 cell line has been characterized in T-flasks both with and without cell attachment. In RPMI 1640 medium supplemented with 10% FBS, the population doubling time of the PC-3 cell line was found to be 25 hours when the cells were attached (which is consistent with the previous results of other investigators). Next, the cell attachment surface was treated with poly 2-hydroxyethylmethacrylate, which completely inhibited cell attachment at the concentration we used. Under the latter conditions, the cells grew in aggregates and were rounded (vs. spread out when attached). These cells had a population doubling time of 39 hours. In contrast to this situation, PC-3 cells grown in the RWV did not form clumps, i.e., they grew as individual cells. We have also found that the LNCaP cell line grew with a population doubling time of 56 hours when attached in tissue culture flasks. Fourth, the glucose, lactate, and amino acid concentrations were determined in the PC-3 cell cultures grown in the RWV and tissue culture flasks as a function of time. It was found that most (>80%) of the glucose was converted to lactate (the dissolved oxygen concentration was not measured, thus we cannot be certain that oxygen was not limited). It was also found that glutamine is the most widely consumed amino acid (only minor amounts of other amino acids were consumed) and that alanine accumulated in the cultures. Fifth, light and electron microscopic (transmission and scanning) morphologic analysis of six human prostate cancer cell lines grown in conventional tissue culture flasks has been completed. This will form the basis for subsequent comparison to growth in the RWV. Our studies into the role of CD44 in prostate cancer invasion and metastasis is ongoing. We have established all of the required techniques for analysis, including (i) flow cytometric analysis of surface expression and western blot for protein level expression, (ii) RT-PCR and northern blot for mRNA level expression, (iii) cytokine modulation of surface and soluble expression, (iv) chondroitinase treatment of tumor specimens and immunohistochemical analysis of chondroitin sulfate side chains, and (v) *in vitro* adhesion and migration assays to determine a mechanistic role for CD44. We have determined the levels of E-cadherin on *in vitro* cell lines, as well as the effect of various cytokines on expression, including GM-CSF.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 2
MS Students: 0
PhD Students: 2

TASK INITIATION: 8/95 **EXPIRATION:** 8/99

PROJECT IDENTIFICATION: 962-23-01-24

NASA CONTRACT NO.: NAG9-824

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Chung, H., Arnold, M., Rhiel, M., and Murhammer, D. Simultaneous measurements of glucose, glutamine, ammonia, lactate, and glutamate in aqueous solutions by near-infrared spectroscopy. *Applied Spectroscopy*, 50, 270-276 (1996)

Cohen, M., Griebeling, T., Aherghotu, C.A., Rokhlin, O., and Ross, J. Cellular adhesion molecules in urologic malignancies. *American Journal of Clinical Pathology*, (In Press).

Riley, M., Rhiel, M., Zhou, X., Arnold, M., and Murhammer, D. Simultaneous measurement of glucose and glutamine in insect cell culture media by near-infrared spectroscopy. *Biotechnology and Bioengineering*, (In Press).

Dissertations

Zhou, X. to Murhammer, D. "Near infrared spectroscopy for monitoring bioreactor components and chemiluminescence sensors for hydrogen peroxide, glucose, and nitric oxide, Ph. D. Thesis, University of Iowa, Iowa City, IA." 1996.

Presentations

Arnold, M. "Optical sensor designs for remote, selective, reliable, and continuous monitoring." First Gordon Conference on Chemical Sensors and Interfacial Design, Colby-Sawyer College, New London, New Hampshire, July 28, 1996.

Arnold, M., Murhammer, D., and Cohen, M. "Continuous, non-invasive monitoring of rotating wall vessels and applications to the study of prostate cancer." Investigators' Working Group Meeting, Microgravity Sciences and Applications Division, NASA, February 23, 1996.

Chung, H. and Arnold, M. "Development of an optical oxygen sensor with a radioluminescent light source." Pittcon'96, Chicago, IL, March 7, 1996.

Rhiel, M., Murhammer, D., Zhou, X., and Arnold, M. "Cell culture process monitoring by NIR spectroscopy." Pittcon'96, Chicago, IL, March 5, 1996.

Rhiel, M., Riley, M., Zhou, M., Arnold, M., and Murhammer, D. "Sensitivity and selectivity of near-infrared spectroscopy methods for process monitoring." AIChE National Meeting, Chicago, IL, November, 1996.

Riley, M., Arnold, M., and Murhammer, D. "Non-invasive measurement of glucose concentrations by near infrared spectroscopy." Biomedical Engineering Society Fall Meeting, State College, Pennsylvania, 1996.

Riley, M., Rhiel, M., Arnold, M., and Murhammer, D. "Monitoring metabolite concentrations in insect and mammalian cell bioreactors by NIR spectroscopy." AIChE National Meeting, Chicago, IL, November, 1996.

Zhou, X., Arnold, M., Murhammer, D., and Rhiel, M. "Feasibility of on-line bioreactor monitoring by near infrared spectroscopy." Federation of Analytical Chemistry and Spectroscopy Societies, Cincinnati, Ohio, October 15, 1995.

Insect-Cell Cultivation in Simulated Microgravity

PRINCIPAL INVESTIGATOR: Prof. Kim O'Connor

Tulane University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

As discussed in the 1995 report on our NASA grant (NAS9-773), we found distinct differences in the growth and metabolic properties of *Spodoptera frugiperda* insect cells cultivated in simulated microgravity within the High Aspect Rotating-Wall Vessel (HARV) as compared to conventional bioreactors such as shaker flasks. These studies were conducted over a 14-day period.

During the first year of the renewed grant the focus of our research has been to extend our comparison of HARV and shaker-flask cultures of *S. frugiperda* cells to stationary phase and death phase, characterizing differences in cell properties and investigating the mechanisms underlying these changes. To this end, the insect cells were cultivated in the HARV and shaker flask for 50 days.

Task Description:

Our current research involves the cell line IE1FB, a clone derived from *S. frugiperda*. In comparing HARV cultures of insect cells with those produced in conventional bioreactors, we selected a shaker flask for the control. Relative to other conventional bioreactors, shaker flasks provide an extremely gentle culturing environment because of its lack of an impeller. Yet, hydrodynamic forces in this control are nearly twice the magnitude of those encountered in the HARV. Differences observed between HARV and shaker cultures of insect cells should be applicable and magnified when comparisons are made between the HARV and more turbulent bioreactors.

Task Significance:

Insect cells are invertebrate animal cells that show great potential as hosts for the commercial production of recombinant proteins. This is a relatively new phenomenon, beginning in the mid-1980's. Since this time, there has been an explosive growth in the number of recombinant proteins that have been expressed in insect cells with less than 10 by 1984 to over 100 by 1990. The reason for this growth is the ease with which recombinant proteins can be expressed in and purified from insect cells relative to mammalian cells.

Recombinant proteins are playing an increasingly greater role in medicine, basic research and agriculture for use as protein therapies, diagnostic agents and insecticides to name a few. The sale of recombinant proteins makes a substantial contribution to the U.S. economic market. In the pharmaceutical industry alone, biotherapies, which are primarily recombinant proteins, generated \$1.2 billion in U.S. sales in 1991 and are predicted to generate nearly \$8.0 billion in 2001.

With current technology, commercial production of recombinant proteins from insect cells is hindered since they are more sensitive to hydrodynamic forces in a bioreactor and have a greater oxygen uptake rate than most vertebrate cells. This combination places severe constraints on cell oxygenation during large-scale cultivation; sufficient oxygen must be transported to the insect cells for respiration without inducing hydrodynamic damage to the cells.

Conventional methods of oxygenation, such as sparging, supply sufficient oxygen but do so by increasing mixing of growth medium and gas flow rate, resulting in cell destruction from hydrodynamic forces in the medium and at the gas/liquid interface.

The HARV provides a low-turbulence environment in which cells grow suspended in culture medium through end-over-end mixing and are oxygenated via a silicon membrane. In this environment, hydrodynamic forces are greatly reduced over those in conventional bioreactors while mass transfer rates for oxygen remain high.

Our research evaluates the potential of the HARV for cultivation of insect cells.

Progress During FY 1996:

In previous research, we developed a methodology to cultivate *S. frugiperda* cells in simulated microgravity within the HARV as described in the 1995 report on our NASA grant.

The initial experiments were conducted over a 14-day period. During this time, both the growth and metabolic profiles in this environment were profoundly different than those obtained from shaker-flask cultures. For example, nutrient consumption and waste production were lower in the HARV than in the shaker-flask control. This may be beneficial to commercial cultivation of insect cells by reducing medium requirements and, thus, reducing cost.

Since the grant began in August 1995, we expanded the cultivation time in the HARV from 14 days to 50 days in order to conduct an in-depth study of *S. frugiperda* cells in stationary and death phase.

In the HARV, the duration of stationary and death phase was greatly extended over that achieved in shaker-flask controls. For both HARV and control cultures, *S. frugiperda* cells grew to concentrations in excess of 1×10^7 viable cells/ml with viabilities greater than 90%. In the HARV, stationary phase was maintained for 9 to 15 days in contrast to 4 to 5 days in the shaker flask. Furthermore, the rate of cell death was reduced in the HARV by at least a factor of 20 relative to the control culture and was characterized with a death rate constant of 0.01 to 0.02 day⁻¹. Beginning in stationary phase and continuing in death phase, there was a significant decrease in population size in the HARV versus an increase in the shaker flask. This phenomenon could represent cell adaption to simulated microgravity and/or a change in the ratio of apoptotic to necrotic cells. Differences observed in this research between the HARV and its control were attributed to a reduction in hydrodynamic forces in the microgravity vessel. The prolonged stationary phase and slower rate of cell death in HARV cultures of *S. frugiperda* cells may be useful in insect-cell cultivation by greatly extending cultivation time. A manuscript describing this research is in press in *Enzyme and Microbial Technology*.

Based on these findings, we have hypothesized that the HARV may alter cell death mechanisms. DNA fragmentation patterns resolved with agarose gel electrophoresis provide initial support for this hypothesis. The gels suggest that shaker-flask cultures were dominated by necrotic cell death, whereas HARV cultures contained a greater percentage of apoptotic cells. We hypothesize that necrosis in the shaker flask was the result of hydrodynamic damage to the cell membrane. Since the magnitude of hydrodynamic forces was less in the HARV, a greater percentage of cells growing in this quiescent environment died by apoptosis.

We are currently characterizing the percentages of viable, early apoptotic, late apoptotic, and necrotic cells in the HARV and shaker flask as a function to time. These different groups can be readily detected by staining the cells with acridine orange and ethidium bromide, two fluorescent DNA binding dyes. These data will be supported with an analysis of DNA fragmentation with flow cytometry. If our hypothesis is correct, we will model the dynamics of the cell population in the HARV and shaker flask, obtaining kinetic constants for the different death mechanisms.

In addition to our work with insect cells, we studied the effects of simulated microgravity on DU 145 human prostate adenocarcinoma cells.

From our previous studies with this cell line, we learned that simulated microgravity significantly alters cell aggressiveness, resulting in a slower growing, more differentiated, and less pliant culture than can be obtained in either a spinner flask or Transwell insert. This research has recently been published in the June, 1996 issue of *Biotechnology and Bioengineering*.

Currently, our focus is to investigate the mechanisms that underlie this phenomenon. During fiscal year 1996, we characterized select regulatory and matrix proteins in aggregates of DU 145 cells grown in simulated microgravity within the HARV, spinner flask, and Transwell insert. For HARV cultures, three-dimensional growth and doubling times were 3 and 1.5 times greater, respectively, than for Transwell cultures. There was a 1.7- to 19-fold increase in staining intensity for (i) transforming growth factor b1 (TGFb1), collagen IV and laminin in HARV cultures and (ii) epidermal growth factor (EGF), EGF receptor, and TGFb receptor in Transwell cultures. Spinner-flask cultures had doubling times identical to HARV cultures but less three-dimensional growth. Their staining intensities often resembled those for Transwell cultures. These results suggest that HARV cultures were the least aggressive in this study. Moreover, they suggest that this change was caused partially by increased three-dimensional growth and was mediated, in part, through EGF and TGFb1 autocrine loops. This work has been submitted to *Tissue*

Engineering. In the manuscript, we discuss the analogy of HARV cultures behaving as a differentiated solid tumor, Transwell cultures — an aggressive invading tumor margin; and spinner-flask cultures, an intermediate between these two extremes.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	1
PhD Students:	2	PhD Degrees:	0

TASK INITIATION: 8/95 EXPIRATION: 7/99

PROJECT IDENTIFICATION: 962-23-01-21

NASA CONTRACT NO.: NAG9-826

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Clejan, S., O'Connor, K.C., Cowger, N.L., Cheles, M.K., Haque, S., and Primavera, A.C. Effects of simulated microgravity on DU 145 human prostate carcinoma cells. *Biotechnol. Bioeng.*, 50, 587-597 (1996).

Cowger, N.L., O'Connor, K.C., and Bivins, J.E. Influence of simulated microgravity on the longevity of insect-cell culture. *Enzyme Microb. Technol.*, In press, (1996).

Cowger, N.L., O'Connor, K.C., and Bivins, J.E. Characterization of microgravity cultures of insect cells in stationary and death phase. *In Vitro Cell. Dev. Biol.*, 32, 37A (1996).

Francis, K.M., O'Connor, K.C., and Spaulding, G.F. Cultivation of fall armyworm ovary cells in simulated microgravity. *In Vitro Cell. Dev. Biol.*, In Press, (1996).

O'Connor, K.C., Enmon, R.M., Dotson, R.S., Primavera, A.C., and Clejan, S. Characterization of autocrine growth factors, their receptors and extracellular matrix present in three-dimensional cultures of DU 145 human prostate carcinoma cells grown in simulated microgravity. *Tissue Eng.*, Submitted, (1996).

O'Connor, K., Rosenzweig, N., and Clejan, S. Simulated microgravity inhibition of in vitro aggressiveness of prostate cancer is accompanied by changes in signal transduction and lipid second messengers. *FASEB J.*, 10, A1396 (1996).

NASA Tech Briefs

O'Connor, K.C. Cultivating insect cells to produce recombinant proteins. *NASA Tech Brief*, 20, 79 (1996).

Books

Francis, K.M., O'Connor, K.C., Blake, D.A., Caldwell, D.R., and Spaulding, G.F. "Growth and structure of corneal tissue in simulated microgravity." 959-963. *Animal Cell Technology: Developments Towards the 21st Century*, Kluwer Academic Publishers, Dordrecht, 1995.

O'Connor, K.C., Enmon, R.M., Primavera, A.C., Dotson, R.S., and Clejan, S. "Characterization of extracellular matrix in three-dimensional cultures of DU 145 human prostate carcinoma cells." *Animal Cell Technology: From Vaccines to Genetic Medicine*. Kluwer Academic Publishers, Dordrecht, In Press, 1996.

Presentations

Cowger, N., O'Connor, K., and Bivins, J. "Characterization of microgravity cultures of insect cells in stationary and death phase." 1996 World Congress on In Vitro Biology: Society for In Vitro Biology, San Francisco, CA, 1996.

Cowger, N., O'Connor, K., and Bivins, J. "Behavior of insect cells during long-term cultivation in simulated microgravity." Annual Meeting of the American Institute of Chemical Engineers, Chicago, IL, 1996.

O'Connor, K., Clejan, S., Cowger, N., Enmon, R., Dotson, R., and Primavera, A. "Effects of simulated microgravity on DU 145 human prostate carcinoma cells." Spring Meeting of the American Chemical Society, New Orleans, LA, 1996.

O'Connor, K., Clejan, S., Cowger, N., Enmon, R., Dotson, R., and Primavera, A. "Effects of simulated microgravity on DU 145 human prostate carcinoma cells." Cancer Association of Greater New Orleans, New Orleans, LA, 1996.

O'Connor, K., Clejan, S., Enmon, R., Rosenzweig, N., Dotson, R., and Primavera, A. "Characterization of autocrine regulatory processes in DU 145 human prostate carcinoma cells." Annual Meeting of the American Institute of Chemical Engineers, Chicago, IL, 1996.

O'Connor, K., Enmon, R., Primavera, A., Dotson, R., and Clejan, S. "Characterization of growth factors and extracellular matrix in three-dimensional cultures of DU 145 human prostate carcinoma cells." Meeting of the European Society for Animal Cell Technology, Vilamoura, Portugal, 1996.

Shear Sensitivities of Human Bone Marrow Cultures

PRINCIPAL INVESTIGATOR: Dr. Bernhard O. Palsson

University of California, San Diego

CO-INVESTIGATORS:

Wang, H.

University of Michigan

Task Objective:

Many studies examine fluid flow and shear stress on cells in culture and attribute changes in cell behavior to shear stress. These studies may overlook the coupled effect of mass transfer and convection of biological factors in a culture, both of which change with flow rate. Our overall objective is to understand the complex interplay between physical processes, such as diffusion, shear stress, and convection on one hand, and biological processes such as secretion and chemoreception on the other, that occur simultaneously in complex primary human tissue cultures. Once these are better understood, we can use such results to determine optimal growth conditions for human cultures, such as bone marrow, in the RWV.

Task Description:

We will proceed in a stepwise fashion, beginning with simple situations, and build towards increased complexity to approach the dynamic conditions that exist in the RWV. These steps are:

1. Develop a model for spherical diffusion to mimic a "solitary" cell.
2. Develop a model for diffusion from a confluent cell layer mimic a "social" cell.
3. Use a numerical simulation to obtain solutions where analytical solutions cannot be obtained.
4. Develop a model for spherical diffusion with fluid flow to determine how the diffusional process is altered.
5. Develop a model for diffusion from a confluent layer of cells with fluid flow.
6. Perform a pilot Fluorescent Resonant Energy Transfer (FRET) experiment using a pair of fluorescent receptors and ligands to test a method of imaging concentrations of biological factors in a tissue culture.
7. Establish a cell line that secretes Green Fluorescent Protein (GFP), derived from the jellyfish *Aequorea Victoria*, as an additional method for imaging concentrations of biological factors in a tissue culture.
8. Observe secreting cells with a confocal microscope equipped with time-lapse capability so that the transients of protein diffusion can be directly observed.
9. Measure concentration gradients of biological factors near cells using a confocal microscope to validate theoretical models.
10. Investigate regions of slow fluid flow in a tissue culture to determine the effect on biological factor concentration.
11. Investigate inoculum cell density effects on biological factor concentration in a 2 x 2 experimental design with high low cell density versus flow/no flow.
12. Begin the process with easy-to-grow cell lines and then try human bone marrow.
13. Determine optimal growth conditions in the RWV.

Task Significance:**Cellular therapies require tissue development ex-vivo**

Cellular therapies promise to become an important therapeutic modality in the near future. They involve the transfusion of primary human cells, either in an autologous or allogenic setting, to render a clinical benefit to the recipient. Many such therapeutic applications rely on the growth of primary cells and tissues *ex vivo*. One challenge that must be met in order for these therapies to succeed is to understand the processes occurring in the *ex vivo* cellular environment so the transfused cell population can be produced in a reliable and efficient manner.

Tissue development requires communication between cells

Tissues are comprised of "functional units", such as the nephron in the kidney and the villi in the small intestine. The functional units of tissues contain many different cell types that continuously communicate with one another through a variety of mechanisms. An important mode of communication is the release of soluble cyto- and

chemokines. These signals lead to the induction of organogenic processes such as cell proliferation, differentiation, and motion. These organogenic processes in turn influence the development of the tissue, including the cell types and numbers that are produced.

Communication is regulated by Physcio-Chemical and Biological processes, understanding their relationship is critical to cellular therapies

When primary cells are aspirated or biopsied and placed in culture they are taken out of their normal physiological environment. They respond by trying to reconstitute tissue function in the environment in which they are placed. If this *ex vivo* environment simulates the *in vivo* condition sufficiently well, partial or full tissue function results. A cell's ability to propagate and receive signals is critical in this process. This mode of communication is both physcio-chemically and biologically regulated. By understanding the complex interplay between these processes, we will be able to make more effective use of *ex vivo* culturing systems and, in turn, develop cellular therapies to their full potential.

The use of the RWV

Partial success has been obtained using standard tissue culture procedures and perfusion bioreactors that are aimed at automating such cultures. Tight cell attachment and tissue growth on a 2D surface characterizes such bioreactor systems. The RWV does not display these characteristics and may be advantageous for bone marrow cultivation.

Progress During FY 1996:

Over the past months following the move of the program to UCSD we have 1) developed a mathematical model for spherical diffusion from cells, 2) developed a mathematical model for diffusion from a sheet of cells, 3) obtained reagents for pilot FRET experiments that will determine the feasibility of direct detection of biological factor concentration gradients, 4) researched procurement of confocal microscope - separately funded, 5) researched uses and sources of Green Fluorescent Protein DNA, and 6) written a draft of a paper based on spherical diffusion model (see 1) above).

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	1
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 11/92 EXPIRATION: 11/97
 PROJECT IDENTIFICATION: 962-23-01-09
 NASA CONTRACT NO.: NAG9-652
 RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Francis, K. and Palsson, B.O. Effective Communication Distances in Complex Cell Cultures are Determined by the Relative Cytokine Secretion and Diffusion Time Constants. In Preparation, (1996).

Kim, B.S. and Palsson, B.O. Clinical Scale Production of Human Hematopoietic Progenitors in a Suspense Bioreactor. Submitted, (1996).

Peng, C.A. and Palsson, B.O. Cell Growth and Differentiation on Feeder Layers is Predicted to be Influenced by Bioreactor Geometry. Biotechnology and Bioengineering, Vol. 50, 479-492 (1996).

Peng, C.A. and Palsson, B.O. Importance of Nonhomogeneous Concentration Distributions Near Walls in Bioreactors for Primary Cell Cultures. Ind. Eng. Chem. Res., Vol. 34, 3239-3245 (1996).

Peng, C.A., Koller, M.R., and Palsson, B.O. Unilineage Model fo Hematopoiesis Predicts Self-Renewal of Stem and Progenitor Cells from Observed Ex Vivo Growth Patterns. Biotechnology and Bioengineering, 52:24-33 (1996).

Microgravity and Immunosuppression: A Ground-Based Model in the Slow Turning Lateral Vessel Bioreactor

PRINCIPAL INVESTIGATOR: Dr. Neal R. Pellis

NASA Johnson Space Center (JSC)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Simulated and true microgravity modulate immune function by affecting lymphocyte locomotion through an intercellular matrix. The objective of this investigation is to determine the nature of the lesion(s) that contribute to the loss of movement in lymphocytes in microgravity. The system is modeled using the bioreactor technology that simulates microgravity for cells.

Task Description:

The investigation addresses three specific aims that encompass the use of the Slow Turning Lateral Vessel (STLV) as a model for microgravity. In the first aim, the basis of the loss of locomotion in the STLV is sought using video and biochemical analysis of the critical components of lymphocyte locomotion. The second seeks the basic mechanisms to be targeted in an attempt to ameliorate the loss of lymphocyte locomotion in the STLV and in microgravity. The third aim is to determine if the loss in locomotion is related to actual decline in immunity.

Task Significance:

The ability of the immune system to function appropriately is predicated on many different cellular activities. A critical aspect is the movement of lymphocytes through interstitium to engage and destroy antigenic stimulus. Both clinostatic rotation and actual microgravity of space inhibit the locomotion of lymphocytes through Type I collagen. Therefore, it is essential to understand how alterations in gravity modify immune function, not only in the context of space travel, but also to apply the microgravity tool to modulate immune function. Knowledge of physical control of cellular movement may enable development of novel strategies to control or promote the inflammatory process.

Progress During FY 1996:

Clinostatic rotation in the STLV inhibits the locomotion of resting lymphocytes through Type I collagen. Activation by polyclonal stimulation increases the proportion of locomotory cells in the STLV. Treatment of lymphocytes with transferrin-iron complex significantly promoted locomotion in stationary and rotated lymphocyte cultures. An immunological adjuvant, lipophilic muramyl-tripeptide (MTP-PE) had similar activity. It is tentatively concluded that each of these processes may result in the production of chemokinetic substances that participate in the locomotory process. Recently we observed that the state of activation of lymphocytes determines their locomotory activity. Polyclonal activation or stationary culture precludes STLV inhibition or locomotion. Furthermore, treatment with phorbol esters and ionomycin ameliorates the STLV induced depression of activation.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 9/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-23-01-38

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Campbell-Washington, J., Craig, J.N., Baker, T., Risin, D., Goodwin, T.J., and Pellis, N.R. Differential display RT-PR analysis and cloning of novel mRNAs expressed in HL-60 promyelocytic cells cultured in simulated microgravity conditions. *FASEB J.*, 10(6), (Abst.) (April 30, 1996).

Cooper, D. and Pellis N.R. Cell-cell and cell-matrix interactions aid mitogen induced T lymphocyte activation in simulated microgravity. *FASEB J.*, 10(6), (Abst.) (April 30, 1996).

Pellis, N.R., Goodwin, T.J., Risin, D., McIntyre, B.W., Pizzini, R.P., Cooper, D., Prewett, T.L., and Spaulding, G.F. Randomization of gravitational vectors inhibits human lymphocyte locomotion through type I collagen. *In Vitro*, (In Press).

Risin, D., Kleinerman, E.S., Umez, Y., Pizzini, P.R., Valch, C.M., and Pellis, N.R. Impairment of lymphocyte locomotion in the tumor microenvironment and the effect of systemic immunotherapy with L-MTP-PE. *Cancer Immunol. Immunother.*, 40:57-64, (1995).

Risin, D., Prewett, T.L. and Pellis, N.R. Suppression of lymphocyte function in microgravity and potential impact on immunosurveillance. Abstracts of the Fifth International Conference on Anticancer Research, October 17-22, 1995, Corfu, Greece. *Anticancer Res.*, Vol 15, Number 5A, 1652 (Abst #72) (Sept-Oct 1995).

Books/Chapters

Pellis, N.R., Ellis, L., and Balch, C.M. "Tumor Biology". In: "Surgery: Scientific Principles and Practice." Philadelphia: JB Lippincott, 1996.

Presentations

Campbell-Washington, J., Craig, J.N., Baker, T., Risin, D., Goodwin, T.J., and Pellis, N.R. "Differential display RT-PCR analysis and cloning of novel mRNAs expressed in HL-60 promyelocytic cells cultured in simulated microgravity conditions." ASBMB/ASIP/AII Joint Meeting, New Orleans, Louisiana, June 6-8, 1996.

Cooper, D. and Pellis, N.R. "Cell-cell and cell-matrix interactions aid mitogen induced T lymphocyte activation in simulated microgravity." ASBMB/ASIP/AII Joint Meeting, New Orleans, Louisiana, June 6-8, 1996.

Jessup, J.M., Goodwin, T.J., Garcia, R., and Pellis, N.R. "STS-70: Flight of EDU-1." NASA Symposium: Cell Culture Bioreactor and Three-Dimensional Culture Studies, World Congress on In Vitro Biology, San Francisco, California, June 25, 1996.

Pellis, N.R. "Establishment of 3-dimensional primary hepatocyte cultures in microgravity environment." Amer. Assoc. for the Study of Liver Diseases, 11/3-11/7/95, Chicago, IL. *Hepatology*, Vol. 22, No. 4, Pt. 2, P. 231A (Abst. #498), 1995.

Pellis, N.R. "Biotechnology and Space Research." University of Houston, Clear Lake, Houston, Texas, November 3, 1995.

Pellis, N.R. "Research Update: Microgravity and Immunosuppression." Gillison-Longbaugh Foundation, Houston, Texas, November 7, 1995.

Pellis, N.R. "Biomedical research in space." Tulare Country Medical Society, Visalia, California, February 16, 1996.

Pellis, N.R. "Microgravity and Immunosuppression: A Ground-based Model in the Slow Turning Lateral Vessel Bioreactor." Investigators Working Group (IWG), Houston, Texas, February 24, 1996.

Pellis, N.R. "Cell Biology in Space." San Jacinto College, Houston, Texas, March 4, 1996.

Microgravity Crystallization of Avian Egg White Ovostatin

PRINCIPAL INVESTIGATOR: Dr. Marc L. Pusey

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Carter, D.

NASA Marshall Space Flight Center (MSFC)

Task Objective:

The research objective is designed to study the protein ovostatin for its suitability as a model protein for protein crystal nucleation and growth mechanisms, the bio-mechanical movements which form the basis of its inhibitory activity, and using it as a means of studying the alpha-2-M group of proteins. Further, the intention is to develop the crystallization conditions to be tried based upon studies of the physico-chemical parameters, such as solubility phase behavior and observed nucleation kinetics. This will be our first demonstration protein for the application of what is being learned about the crystal growth of macromolecules.

Task Description:

The study of ovostatin is of interest for several reasons. This protein is attractive as a model for protein crystal nucleation and growth studies. Crystals can be easily and rapidly grown in bulk solution. With a minimum step height of 25-34 nm (the molecular dimensions), surface features should be readily detectable in real-time using interferometric or atomic force microscopy techniques, allowing direct observation of the crystal growth process. The large size would facilitate protein crystal nucleation studies using light scattering methods. Practically, ovostatin can be easily purified in large quantities, requiring about six dozen hen egg whites/gram of protein. Material purified has been stable for prolonged periods (over four months) during crystallization trials and has been kept for over one year as a lyophilized powder. Finally, there is the similarity between it and alpha-2-macroglobulin. Currently, the only structural information for this group of proteins comes from electron microscopy studies of isolated molecules.

Task 1: Preparation of ovostatin for use in experiments. Large scale protein purification will be continuous for the duration of the project. This material will be used to establish the reference ground-based crystal quality against which future flight crystals will be measured. Ovostatin prepared in this laboratory will be made freely available to other researchers wishing to study it.

Task 2: Screening of ovostatin crystallization conditions. The best crystallization conditions determined at this time will be used for future flight experiment(s). These conditions will then be used for the final solubility diagram determinations to be used in designing the flight experiments.

Task 3: Establishing baseline crystal quality. Multiple data sets will be acquired using the x-ray diffractometer. These will be used to establish the baseline ground-grown crystal quality.

Task 4: Studies of ovostatin. These will last for the duration of this project. These will be done using the instrumentation developed in the laboratory for the study of the protein crystal nucleation and growth processes.

Task Significance:

Any knowledge gained about ovostatin based on crystal structure analysis would advance the overall knowledge of this family of proteins.

Progress During FY 1996:

Previous microgravity protein crystal growth experiments have used vapor diffusion, free interface diffusion, and dialysis techniques with most being done using vapor diffusion. Littke and John, using free interface diffusion, reported a 10^3 volume increase for beta-Galactosidase over crystals grown on Earth. In vapor diffusion experiments, at least three proteins have shown significantly improved diffraction resolution over any of the crystals grown on Earth, despite the fact that because of short flight durations crystallization conditions have had to be optimized for rapid nucleation and growth (i.e., the temporal conditions were more favorable for lower quality crystals). Current

Isolation of the Flow, Growth and Nucleation Rate, and Microgravity Effects on Protein Crystal Growth

PRINCIPAL INVESTIGATOR: Dr. Marc L. Pusey

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

No Co-ITs Assigned to this Task

Task Objective:

The purpose of these studies is to determine how μg affects the protein crystal growth process and how that effect can be optimized for the production of higher diffraction quality protein crystals. In pursuit of this goal, the research will comprise a ground and, eventually, a g-based program. The research will consist of:

- the development of new proteins for use as models in protein crystal growth studies;
- determinations of protein solubilities as a function of solution parameters;
- the determination of protein crystal nucleation rates;
- the effects of low velocity solution flow on protein crystal nucleation and growth rates;
- the effects of low velocity solution flow on protein-protein and protein-solvent interactions; and,
- the effects of protein crystal nucleation and growth rates on Earth and in μg on crystal diffraction quality.

At the conclusion of this effort several new proteins will have been developed as models for protein crystal growth. This will entail acquiring a detailed background knowledge about their crystallization conditions and solubility behavior, to a level of detail approximating that currently available for hen egg-white lysozyme. This data will be invaluable for the subsequent research to be carried out in this and other laboratories.

Task Description:

For the first year, the efforts will be centered upon developing methods of measuring crystal nucleation rates and reconciling these methods with each other and with more traditional "bulk solution" type measurements. Instrumentation will be acquired to build a means of following the aggregation, by light scattering, scintillation, and/or fluorescence methods, along a low velocity flow cell. Measurements will be made of crystal growth rates in a flowing solution. The effects of variations in the nucleation and growth rate on lysozyme crystal quality will be determined, based upon experiments done with a long duration dialysis system developed in this laboratory (McDUCK, or Multiple-chamber Dialysis Unit for Crystallization Kinetics). We will also begin the screening process for development of several new proteins as potential candidate model proteins for use in protein crystal growth studies.

Task Significance:

Evidence shows that high purity and a typically narrow range of solution conditions are important to the growth of high x-ray diffraction quality protein crystals. Intuitively, one would assume that careful control of the processes, resulting in the slow growth of carefully nucleated crystals, would result in the highest quality crystals. To date this has not been demonstrated and the comparative effects of nucleation rate, growth rate, and μg on the obtained protein crystal quality are not known. Also absent are any clear explanations for the effects of solution flow on protein crystal growth, often cited as the rationale for the use of μg . This research will show, using several model proteins, how each factor (i.e., nucleation rate, growth rate, solution flow, and μg) affects protein crystal growth. These results can then be incorporated into the subsequent design of protein crystal growth systems for use both on Earth and in μg .

Progress During FY 1996:

Ovalbumin and Ovalbumin have been prepared in large quantities (ca 1 Kg each) directly from fresh eggs, and preliminary crystallization trials have been initiated to determine "good" crystallization conditions. The solubility of a-chymotrypsinogen is now being determined at pH 6.8 in preparation for nucleation rate studies with this protein.

experiences are that ovostatin crystals nucleate and finish growing within a one- to three-day period. The process will have to be slowed down to fit better within the timeframe for a typical microgravity PCC experiment, as opposed to the usual case where the crystal growth process must be speeded up. Based on the ovostatin crystal results have now shown that ovostatin gives better yields and more reproducible crystallization when purified from freshly laid eggs. However, no improvements have been found in the diffraction data.

Ovostatin purified in this laboratory has now been supplied to four other research groups as a test material. Dr. William Wilson (Mississippi State University) has found a dramatic dimerization-tetramerization behavior at low ionic strength. This has led us to an investigation of ovostatin activity vs. structure which has been carried out by a mummery faculty (Dr. D. Moriarty, UAH). Ovostatin crystallizability has been found to be very sensitive to the purification procedure and materials employed. We are currently supplying ovostatin to the laboratory of Dr. David Blow (Imperial College) for extensive crystallization trials which we hope will lead to a preliminary structural determination. However, the protein sent to Imperial College has yet to crystallize, even when material from the same preparation gives crystals in our laboratory. Also, we have yet to find any new crystallization conditions for ovostatin beyond those first described in the initial proposal.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1
MS Students:	0
PhD Students:	0
TASK INITIATION: 1/93 EXPIRATION: 1/96	
PROJECT IDENTIFICATION: 962-23-08-26	
NASA CONTRACT NO.: NAG8-984	
RESPONSIBLE CENTER: MSFC	

Preliminary nucleation rate measurements with lysozyme, whereby the percentage of soluble solute is determined over time, have not been highly reproducible. Also, the smallest crystal sizes detectable by this method are in the $\geq 1 - 10 \mu\text{m}$ range, making extrapolation back to the (postulated) 10 - 30 nm sized critical nucleus risky at best. We are now investigating the use of particle sizing technologies (i.e., a Coulter counter), forward light scattering, and fluorescence to more accurately follow nuclei growth in the $\sim 50 - 1000 \text{ nm}$ size range.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/95 EXPIRATION: 6/99

PROJECT IDENTIFICATION: 962-23-08-38

RESPONSIBLE CENTER: MSFC

Stem Cell Expansion in Rotating Bioreactors

PRINCIPAL INVESTIGATOR: Dr. Peter J. Quesenberry

University of Massachusetts

CO-INVESTIGATORS:

Peters, S.

University of Massachusetts Medical Center

Stein, G.

University of Massachusetts Medical Center

Task Objective:

Task #1: Develop improved methods for cytokine-supported *in vitro* expansion or maintenance of engrafting lympho-hematopoietic progenitor/stem cells using the non-shear rotating three-dimensional culture vehicles developed within the NASA research program.

Task #2: Evaluate the culture of purified stem cell populations in the non-shear rotating three-dimensional culture vehicles and compare this with conventional culture vehicles.

Task #3: Determine if a co-culture of isolated irradiated stromal cells or a stromal cell line in the non-shear rotating three-dimensional culture vehicles would improve expansion of stem cells and maintenance of primitive engrafting stem cells.

Taks #4: Evaluate the effects of teflon versus Pexiglass rotation three-dimensional culture vehicles.

Task Description:

For Task #1, we have previously found that cytokine exposure in conventional culture vehicles results in expansion of progenitor cells assayed *in vitro*, and induction of cell cycle progression but the development of a profound defect in engraftment in *in vivo* transplantation models. In our first series of experiments, we will compare conventional culture vehicles to the non-shear rotating three-dimensional culture vehicles for their ability to support both *in vitro* progenitor cells and *in vivo* engrafting cells *in vitro* after exposure to a variety of cytokines including Interleukin-3, Interleukin-6, steel factor, GM-CSF, basic fibroblast growth factor, and Interleukin-1 in various combinations. We will carry out cytokine dose response and time-course evaluate the impact of various cell concentrations, and we will monitor *in vitro* progenitors, their cell cycle status, and engrafting ability. In all of the studies in Task Description #1, whole unseparated murine marrow cells will be cultured. Further, in these experiments, we will assess cytokines in optimal doses for their capacity to expand stem cells *in vitro*, and we will also access different conditions and different cytokine doses for their ability to maintain without induced cell proliferation progenitor/stem cells *in vitro*. These later studies are particularly important. We feel that this may be the culture condition in which engrafting stem cells can be maintained and induction of cycling may impair engraftment. There are many important considerations with regard to the culture of hematopoietic stem cells *in vitro* and approaches to expand stem cell populations. As noted above, our data suggests that cycle activation actually prevents cells from engrafting. However, cycle activation is necessary for expansion of stem cell populations and for retroviral integration in various gene therapy approaches. Therefore, a very important aspect of these studies would be to determine whether stem cells can be induced to expand with associated proliferation and activation of cell cycle. Then this state would be reversed so that an expanded population of stem cells or a gene-carrying population of stem cells may then return to the phenotype of a primitive engrafting stem cell. Accordingly, we will assess various conditions to see if we can reverse the cytokine-induced engraftment defect. Once again, we will compare the non-shear rotating three-dimensional culture vehicles with standard tissue culture flasks. In these experiments, stem cells will be induced to cycle by cytokine exposure, and these populations will then be subjected to either growth in selected low levels of cytokines, hematopoietic stem cell inhibitors such as transforming growth factor beta, or growth on various stromal populations. The goal here would be to induce quiescence in the previously stimulated stem cell populations, and in these studies we will assess the cells for cycle status, progenitor content, and an ability to engraft in *in vivo* models.

Task #2 is as outlined under #1 for whole marrow, but will be carried out on highly purified populations of murine hematopoietic stem cells. Purifications will consist of depleting lineage-positive cells and then selecting cells

which stain very weakly with the dyes Rhodamine and Hoescht. Alternative purifications utilizing Sca antigen or c-Kit are also possible. The assessment of growth and comparison between systems will be as described in Task Description #1.

Task #3 stromal cells will be established in the culture vehicles and then co-cultured with either whole marrow or purified marrow cells. Outcomes would be assessed as outlined under Task Description #1.

Task #4 will evaluate task descriptions 1-3 utilizing the newly designed (at UMMC) teflon rotating, three-dimensional culture vehicles and compare results with those obtained with the conventional Plexiglass cultures.

Task Significance:

Task #1: Successful accomplishment of this Task Objective could lead to superior methods of maintaining hematopoietic stem cells *in vitro* in various proliferative states. This in turn could form a basis for more effective approaches to marrow transplantation and to gene therapy.

Task #2 : The accomplishment of the goals outlined in Task Objective #1, but utilizing purified hematopoietic stem cells, would both open insights into basic stem cell biology and potentially reduce costs in marrow expansion and gene therapy approaches substantially making developed technology much more feasible for clinical application.

Task #3: It is possible that superior results with regard to stem cell maintenance and gene transfer will be obtained in the presence of stromal cell co-culture using the non-shear rotating three-dimensional culture vehicles. Success here would, again, increase efficacy of approaches for both marrow transplant and gene therapy.

Task #4: We may be able to obtain far superior culture yields using the teflon device. This, in turn, would greatly facilitate our studies and potentially yield therapeutic cultures to expand stem cells and for gene therapy.

Progress During FY 1996:

We have now obtained the cylindrical cell culture vessel and have begun our preliminary experiments with the culture vessel. We have not gone through a full detoxification and conditioning of the vessel. We are presently assessing growth of WEHI (a leukemia mouse cell line) cells in the vehicle. We are assessing the growth of WEHI cells in RPMI-1640 with 10% fetal calf serum. The initial experiments are without antibiotics. We initiated cultures with a total of 5.2×10^6 cells in approximately 80 ml. After two days of growth, we obtained 138 million cells in the same volume. Viability of the initial starting cells was 85.6% and after two days was 88.5%. Due to the machine being inadvertently shut off, we also were able to evaluate non-rotary conditions briefly and found that we could resuspend the cells and obtain good ongoing viability. We are at present obtaining micro-carrier beads to initiate co-culture operations and have ordered two more vessels in order to begin comparisons with multiple conditions in the rotary vessels and with stationary flask cultures.

New progress includes enhanced growth in the newly designed teflon rotator culture as compared to conventional Plexiglass rotating cultures or rotation of teflon bottle cultures.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/95 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 962-23-01-20

NASA CONTRACT No.: NAG9-819

RESPONSIBLE CENTER: JSC

Study of Crystallization and Solution Properties of Redesigned Protein Surfaces

PRINCIPAL INVESTIGATOR: Dr. David C. Richardson

Duke University Medical Center

CO-INVESTIGATORS:

Gernert, K.
Richardson, J.Emory University
Duke University Medical Center**Task Objective:**

The objective of this work is to determine what combinations of protein surface features and solution factors best promote the growth of highly ordered protein crystals and to seek strategies for improving control over the process. The experiment design is to make detailed analysis of crystal contacts in Cytochrome B562, construct a planned series of mutations at those crystal contacts, study crystal growth and solubility properties of the mutant proteins, and study resultant crystal order. We will use the results to further refine analyses, hypothesis, and test mutants.

Task Description:

High-resolution x-ray crystal structures of proteins are the backbone of academic and industrial research efforts to understand and control the detailed functional properties of these important molecules. Many such studies are stymied, either by lack of crystals altogether or by crystals whose degree of order is inadequate to show details at the level of resolution needed.

Two sets of factors jointly influence the growth of ordered protein crystals: the atomic-level details of the protein surface, including flexibility and bound waters; and the solution conditions, including concentration and identity of precipitants and other components, pH and ionic strength, temperature, interactions at solid or liquid interfaces, vibration, convection currents, etc. Traditionally, the protein surface was not variable except by trying different species, and the only strategy for solution conditions was simply trying as many variations as possible. The most general conclusion was that what worked for one protein was likely to be different than what worked for another. Recently, however, there has been support and encouragement, largely led by NASA, for scientific study of the process of crystallization. The most notable single result so far has been the demonstration that growth in microgravity can produce significantly better-ordered crystals for many proteins, presumably because of the absence of convection currents at the crystal surface. The absence of convective currents, in turn, allows for the increased effect of random diffusion of the protein molecules at the crystal surface and for the increased effective binding energy of the protein molecule to the growing crystal. Both of these are presumed to lead to more accurate and more stable attachment of the protein molecules to the crystal, and thus a better-ordered crystal.

Three-to-four mutants will be studied per year. Each study will involve computer-aided graphics studies of crystal contacts and design of mutants, genetic engineering of mutants, protein purification, crystallization experiments, crystal solubility determinations, face growth rate measurements, calorimetric measurements of crystal growth, and evaluation of crystal diffraction.

Task Significance:

The research aims are to contribute to the scientific understanding and the practical improvement of protein crystal growth by tying together a series of designed mutations at known crystal contacts with the changes in crystallization behavior and parameters. There are several logical levels at which the results of this research should be useful.

A research study of the relative strengths of the binding of protein molecules into their crystal is important for understanding which factors are improved in microgravity, whether the growth cessation phenomena can be alleviated in normal gravity, and how changes in crystal contacts can improve the overall order of protein crystals. A detailed study of protein crystal contacts and their specific effects may also help in the future to sort out influences on nucleation of protein crystals versus later growth. This research is designed to collect two overlapping but distinct types of information: what specific side chain changes will strengthen or weaken a contact for a particular crystallization media; and what contact strength is optimum, relative both to the other contacts and

to the diffusion and convection conditions. Such information will surely aid in future rational control of the crystallization process. Crystal contacts are one type of protein-protein interaction. Related work in this laboratory studies the full range of such interactions with the eventual goal of designing and controlling protein structure formation as well as crystallization.

Progress During FY 1996:

There has been continued success in growing diffraction quality crystals of Cytochrome B562 with various mutations in one of the crystal molecular contact loops (E 81, G 82, K 83 ; thus B562-EGK is native). However, the crystals are in a variety of space groups and a matched set of native and mutant proteins in the same space group has not been found. Comparison of mutants that crystallize in the same space group is now being done. Data collection was hindered while the X-ray Area Detector System was moved to the new Resource Center and much difficulty was encountered bringing it back up to speed. However, two good and complete data sets were collected from space group C2221 crystals of B562-LAA and four such data sets for B562-SLS. Molecular replacement trials on some of the individual data sets in turn has so far not yielded satisfactory results. Two molecules are expected in the asymmetric unit. Using a single molecule of wild type B562 as the model failed to find non-overlapping solutions. Attempts to use a dimer as the model, based on the wild type crystal associations, has not produced a significant solution. Data set quality is probably not the limiting factor; rather, at least for the dimer trials, it is probable that these mutations perturb the crystal contacts more than was intended. Different molecular replacement strategies and programs are now being employed.

Analysis of molecular contacts and protein interior packing has had a real break-through with the development of significantly better computer tools to characterize "goodness of fit." Small probe contact dots show the need for explicit hydrogens in modeling contacts, and emphasize the importance of studying very high resolution structures to learn the basics of contact design.

STUDENTS FUNDED UNDER RESEARCH:				TASK INITIATION: 8/93		EXPIRATION: 8/96	
BS Students:	3	BS Degrees:	2	PROJECT IDENTIFICATION: 962-23-08-22			
MS Students:	0	MS Degrees:	0	NASA CONTRACT NO.: NAG8-966			
PhD Students:	0	PhD Degrees:	1	RESPONSIBLE CENTER: MSFC			

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Gernert, K.M., Thomas, B.D., Plurad, J.C., Richardson, J.S., Richardson, D.C., and Bergman, L.D. "Puzzle Pieces Defined: Locating Common Packing Units in Tertiary Protein Contacts." Proceedings of Pacific Symposium on Biocomputing, January 1996.

Presentations

Richardson, J.S., Richardson, D.C., LaBean, T.H., Gernert, K.M., and Word, M.J. "The Problem of Unique vs. Approximate Structures in Protein Design (invited lecture)." International Conference on Protein Folding and Design, National Institutes of Health, Bethesda, Maryland, April 23-26, 1996.

Richardson, J.S., Richardson, D.C., LaBean, T.H., Gernert, K.M., and Word, M.J. "The Problem of Unique vs. Approximate Structures in Protein Design (poster presentation)." The Johns Hopkins Protein Folding Meeting, Coolfont, Berkeley Springs, West Virginia, March 16-19, 1996.

Convective Flow Effects on Protein Crystal Growth and Diffraction Resolution

PRINCIPAL INVESTIGATOR: Prof. Franz E. Rosenberger

University of Alabama, Huntsville

Co-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This research aims at developing a detailed understanding of:

- the nucleation and growth mechanisms involved in the crystallization of globular proteins;
- the formation mechanisms of structural and compositional nonuniformities (defects) in protein crystals and their dependence on growth conditions; and,
- the dependence of x-ray diffraction resolution of protein crystals on defect types and concentrations and, thus, on crystallization conditions.

Task Description:

We seek to establish, for select proteins, a correlation of well-defined solution conditions (purity, pH, buffer, precipitant, supersaturation, temperature, and bulk transport) with nucleation and growth behavior during crystallization, and the x-ray diffraction resolution of the resulting crystals.

Towards the above goals we are pursuing the following tasks:

- Characterization of the purity of protein solutions by gel electrophoresis, immunoblotting with comparison to authentic protein standards, and Fast Protein Liquid Chromatography (FPLC).
- Preparation of highly homogeneous protein samples by FPLC.
- Studies of protein interactions and aggregation in under- and supersaturated solutions by static and dynamic light scattering.
- Determinations of the precipitant and protein impurity repartitioning between solutions and growing protein crystals, using atomic absorption and optical spectroscopy, ion selective potentiometry, and gel electrophoresis.
- *In situ* studies of the protein growth morphology and kinetics, with and without forced solution flow, by high-resolution microscopic interferometry.
- Numerical modeling of diffusive-convective mass and momentum transport, and the resulting interface morphology, in geometries characteristic of protein crystallization on Earth and in space, using experimentally determined precipitant repartitioning and growth kinetics data.
- Measurements of the kinematic viscosity of supersaturated protein solutions, with a capillary flow technique, in support of the modeling efforts.
- Measurements of the dependence of the refractive index of solutions on salt and protein concentration, in support of the light scattering studies.
- Measurements of protein solubilities as a function of precipitant concentration, pH and temperature, using a miniaturized optical scintillation technique.
- Characterization of the structural quality of selected crystals by x-ray diffraction and topography to reveal the influence of kinetics and transport effects.

Task Significance:

The pharmaceutical industry needs protein structure information to facilitate rational drug design. However, many of the currently available protein crystals are too imperfect to yield detailed structure information. The reasons for this low crystal perfection are not well understood. Interestingly, crystallization experiments in space have led to significant improvements in crystal perfection for some proteins. Again, the physical mechanisms for this are not clear. Our research aims at clarifying the connection between the magnitude of gravity present during protein crystallization and the resulting crystal quality. This insight is expected to lead to the design of protein crystal growth techniques that result in larger and more perfect crystals.

Progress During FY 1996:

Lysozyme crystallization experiments were performed, in which the initial supersaturation, NaCl concentration, protein purity level and crystallized fraction were varied. Lysozyme and protein impurities, as well as sodium and chloride, were independently determined in the initial solution, supernatant and crystals. The segregation coefficient for Na⁺ and Cl⁻ were found to be independent of the supersaturation and NaCl concentration, and decreased with crystallized fraction/crystal size. Numerical evaluation of the extensive body of data, based on a nucleation-growth/repartitioning model, suggest a core of about 40 μm in which salt is incorporated in much greater concentrations than during later growth. Small crystals containing higher amounts of NaCl also had higher protein impurity contents. This suggests that the excess salt is associated with the protein impurities in the core. X-ray topography revealed strain fields in the crystals' centers comparable in size to the inferred core. The growth rate of crystals smaller than 30-40 μm size were consistently 1.5-2 times lower than those of larger crystals, presumably due to higher chemical potentials in the core.

The growth morphology and kinetics of lysozyme crystal facets were investigated by *in situ* high-resolution interferometry. The protein composition of the growth solution was characterized by fast protein liquid chromatography and gel electrophoresis. In relative pure solutions, the facets exhibited depressions with lower vicinal slope at their edges. In solutions with $\leq 1\%$ of protein impurities that were found to be incorporated into the crystal, the depressions had higher vicinal slope at the edge than at the center of the facet. Since these deviations from planarity increased with crystal size and growth rate, we tentatively assumed that they reflect the bulk-transport caused nonuniformity of nutrient and impurities about a faceted crystal. This supposition was confirmed by model calculations, in which the diffusive bulk transport was coupled with the interfacial step motion. Using experimentally determined transport parameters and step kinetics coefficients, the experimentally observed interface shapes were quantitatively reproduced.

Multi-angle static and dynamic light scattering studies of lysozyme solutions were performed. The Rayleigh ratio and the collective diffusivity were determined as functions of both protein concentration and salt concentration with two different salts. At low salt concentrations the "relative scattering intensity" decreased and the diffusivity increased with protein concentration, compared to the values for a monomeric, ideal solution. With increasing salt concentration, these trends eventually reversed. These observations reflect changes in the protein interactions, in response to the increased salt screening, from net repulsion to net attraction. This invalidates the numerous claims of prenucleation aggregate formation in lysozyme solutions, which were based on an assumed ideal solution behavior.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 2/93 EXPIRATION: 1/96

PROJECT IDENTIFICATION: 962-23-08-23

NASA CONTRACT NO.: NAG8-116

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Lin, H., Vekilov, P.G., and Rosenberger, F. Facet morphology response to nonuniformities in nutrient and impurity supply. II. Numerical modeling. *J. Crystal Growth*, vol. 158, 552-559 (1996).

Vekilov, P.G., Monaco, L.A., and Rosenberger, F. Facet morphology response to nonuniformities in nutrient and impurity supply. I. Experiments and interpretation. *J. Crystal Growth*, vol. 156, 267-278 (1995).

Presentations

Muschol, M., and Rosenberger, F. "Absence of prenucleation aggregation in lysozyme solutions - Static and dynamic light scattering results." Sixth International Conference on Crystallization of Biological Macromolecules, Hiroshima, Japan, November 1995.

Rosenberger, F. "Nucleation and crystallization of globular proteins - what do we know and what is missing?" Sixth International Conference on Crystallization of Biological Macromolecules, Hiroshima, Japan, November 1995.

Vekilov, P.G., and Rosenberger, F. "Impurities, growth layer sources and kinetics fluctuations in the growth of lysozyme crystals."

Vekilov, P.G., Monaco, L.A., Thomas, B.R., Stojanoff, V., and Rosenberger, F. "Impurity- and salt-rich coring in lysozyme crystals." Sixth International Conference on Crystallization of Biological Macromolecules, Hiroshima, Japan, November 1995.

Nucleation and Convection Effects in Protein Crystal Growth

PRINCIPAL INVESTIGATOR: Prof. Franz E. Rosenberger

University of Alabama, Huntsville

CO-INVESTIGATORS:

Vekilov, P.

University of Alabama, Huntsville (UAH)

Task Objective:

The objectives of this research are:

- understanding of the nucleation and crystal growth mechanisms to facilitate a rational approach to protein crystallization;
- determination of the factors that currently limit the x-ray diffraction resolution of protein crystals, and their correlation to crystallization conditions; and,
- development of novel technologies to study and monitor protein crystal nucleation and growth processes, in order to increase the reproducibility and yield of protein crystallization.

Task Description:

We will study the aggregation state in purified, compositionally characterized, under- and supersaturated protein solutions to identify the conditions leading to the formation of crystalline nuclei versus undesirable precipitates. For this task, we are developing a novel methodology/instrumentation for simultaneous multiangle light scattering (SMALS) studies and will apply it to select proteins. The SMALS approach will allow for unambiguous aggregation studies to be conducted at the high supersaturations typical of protein crystallization processes.

We will study the effects of defined solute and impurity transport on morphology and kinetics in protein crystallization and on resulting crystal perfection so that we may test our hypothesis that the limited structural perfection of Earth (and some space) grown crystals is partly due to instabilities in the transport and interfacial processes involved. The growth morphology of select, well characterized proteins, will be monitored by high-resolution, *in situ* interferometry for a wide range of crystallization conditions. In particular, we will study the effects of forced solution flow/convection on kinetics and structural perfection. The structural quality of crystals will be evaluated by x-ray diffraction and topography.

Task Significance:

The pharmaceutical industry needs protein structure information to facilitate rational drug design. However, many of the currently available protein crystals are too imperfect to yield detailed structure information. The reasons for this low crystal perfection are not well understood. Interestingly, crystallization experiments in space have led to significant improvements in crystal perfection for some proteins. Again, the physical mechanisms for this are not clear. Our research aims at clarifying the connection between the magnitude of gravity present during protein crystallization and the resulting crystal quality. This insight is expected to lead to the design of protein crystal growth techniques that result in larger and more perfect crystals.

Progress During FY 1996:

The novel instrumentation for simultaneous multiangle light scattering (SMALS) studies has been designed, and the acquisition/machining of all components has been completed. Assembly and alignment of the unit has begun.

Protein heterogeneities in three commercial hen egg white lysozyme (HEWL) preparations were identified and quantified by SDS PAGE with enhanced silver staining, reversed Fast Protein Liquid Chromatography (FPLC) and immunoblotting with comparison to authentic protein standards. Depending on the source, the contaminating proteins totaled 1-6% (w/w) and consisted of ovotransferrin, ovalbumin, HEWL dimers, and polypeptides with approximate Mr of 39 and 18 kD. Furthermore, we have obtained gram quantities of electrophoretically homogeneous (> 99.9% w/w) HEWL by single step semi-preparative scale cation exchange FPLC with a yield of about 50%.

In situ high-resolution interferometry on horizontal facets of the protein lysozyme reveal that under steady bulk transport conditions the local growth rate R , vicinal slope p and tangential (step) velocity v fluctuate by up to 80% of their average values. The major excursions in R are associated with the formation of lattice defects (striations). The time scale of the fluctuations, which occur through the formation of step bunches (macrosteps), is of the order of 10 min. The fluctuation amplitude of R increases with growth rate (supersaturation) and crystal size. Furthermore, step bunches moving across the interface in the direction or opposite to the buoyancy-driven convective flow increase or decrease in height, respectively. This is in agreement with analytical treatments of the interaction of moving steps with solution flow. We show that, in general, the system-dependent kinetic Peclet number, Pe , i.e., the relative weight of bulk transport and interface kinetics in the control of the growth process, governs the step bunching dynamics. This provides, for the first time, a rationale for system-dependent advantages as well as disadvantages of reduced gravity conditions for (protein) crystallization.

Growth induced defects in lysozyme crystals were studied by white beam and monochromatic x-ray topography at the National Synchrotron Light Source at the Brookhaven National Laboratory. A variety of defects were observed. The topographic methods were non-destructive to the extent that traditional diffraction data collection could be performed to high resolution after topography. It was found that the defect density depends on the purity of the solution and the stability of the temperature during crystal growth. In addition, crystals with fewer defects showed lower mosaicity and higher diffraction resolution.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 7/95 EXPIRATION: 7/98

PROJECT IDENTIFICATION: 962-23-08-43

NASA CONTRACT NO.: NAG8-116

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Muschol, M., and Rosenberger, F. Interactions in undersaturated and supersaturated lysozyme solutions: Static and dynamic light scattering results. *J. Chem. Phys.*, vol. 103, 10424-10432 (1995).

Rosenberger, F. Protein crystallization. *J. Crystal Growth*, vol. 166, 40-54 (1996).

Thomas, B.R., Vekilov, P.G., and Rosenberger, F. Heterogeneity determination and purification of commercial hen egg white lysozyme. *Acta Cryst. D*, vol. 52, 776-784 (1996).

Vekilov, P.G., and Rosenberger, F. Dependence of lysozyme growth kinetics on step sources and impurities. *J. Crystal Growth*, vol. 158, 540-551 (1996).

Vekilov, P., Monaco, L.A., Thomas, B.R., Stojanoff, V., and Rosenberger, F. Repartitioning of NaCl and protein impurities in lysozyme crystallization. *Acta Cryst. D*, vol. 52, 785-798 (1996).

Presentations

Muschol, M., and Rosenberger, F. "Light scattering investigation of phase transitions in lysozyme solutions." International Laser Light Scattering Symposium, Hong Kong, July 1996.

Muschol, M., and Rosenberger, F. "Is the shape of phase diagrams for globular proteins universal?" Photon Correlation and Scattering Topical Meeting, Capri, Italy, August 1996.

Muschol, M., and Rosenberger, F. "Liquid phase separation in lysozyme." Workshop on Response Surface Methods in Protein Crystallization, Univ. of North Carolina, Chapel Hill, June 1996.

Rosenberger, F. "Protein crystallization." Sixth Eastern Regional Conference on Crystal Growth, Atlantic City, New Jersey, October 1995.

Rosenberger, F. "Interaction between bulk transport and interface kinetics in crystal growth from solutions." Second European Symposium on Fluids in Space, Naples, Italy, April 1996.

Rosenberger, F. "Physical chemistry of globular protein crystallization." Gordon Research Conference on Diffraction Methods in Molecular Biology, Proctor Academy, Andover, New Hampshire, June 1996.

Thomas, B.R., and Rosenberger, F. "Heterogeneity determination and purification of commercial hen egg white lysozyme." Protein Crystal Growth Conference, Panama City, Florida, April 1996.

Vekilov, P.G., Alexander, J.I.D., and Rosenberger, F. "Unsteady dynamics of layer growth in the mixed kinetics-bulk transport regime." Tenth American Conference on Crystal Growth, Vail, Colorado, August 1996.

Vekilov, P.G., and Rosenberger, F. "New factors for protein crystal perfection on Earth and under reduced gravity." Protein Crystal Growth Conference, Panama City, Florida, April 1996.

Enhancement of Cell Function in Culture by Controlled Aggregation Under Microgravity Conditions

PRINCIPAL INVESTIGATOR: Prof. W. M. Saltzman

Cornell University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Cell-cell contact within tissues is fundamental to the regulation of cell differentiation and function. Cell aggregates, formed *in vitro* and maintained in culture, have been shown to maintain many of the functions of the native tissue. The main objectives of this program are: i) development of methods for controlling cell aggregation using bioactive polymers and polymer microspheres and ii) systematic study of the function and behavior of suitably aggregated cells in culture. The discovery of new methods for improving cell growth and function in culture is critical to the development of hybrid artificial internal organs and mammalian cell bioreactors.

Task Description:

To achieve these goals, we have formulated the following specific objectives for a three-year period of study:

Objective 1: Synthesis of water soluble polymers for controlling cell aggregation. We will synthesize water soluble polymers with bioactive groups that are specifically recognized by certain cells and use these multifunctional polymers as molecular nuclei to initiate and control cell aggregation. We will use these polymers to control aggregation by adding them to gently agitated or quiescent suspensions of single cells; this technique will produce small cellular aggregates (<10 cells, diameter <100 μm). By altering the properties of the polymers and the conditions of aggregation, we will identify approaches for obtaining cell aggregates of different size, polydispersity, and morphology. We have demonstrated the feasibility of this approach using N-acetyl glucosamine (specific for chicken hepatocytes) attached to vinyl polymers.

Objective 2: Fabrication of polymer microspheres for carrier-assisted cell aggregation. We will fabricate microspheres containing encapsulated, soluble mediators of cell growth and function. We will use the microspheres to create larger aggregates with a central polymer core. We have also demonstrated the feasibility of this approach using microspheres composed of vinyl polymers and cultured hypatocytes.

Objective 3: Development of methods for culturing cell aggregates under unit gravity. In preliminary studies, we have encapsulated hepatocytes and hepatocyte aggregates within gels of type I collagen, cultured these encapsulated cells, and examined subsequent cell growth, function, and viability. We will test gels of collagen under different hydration conditions to find an optimal experimental system for maintaining cells in an aggregated and suspended state in the laboratory. The gels will be used to suspend aggregates created with water-soluble polymers and microspheres. To develop model culture systems representing both liver and neuronal tissues, we will use primary cultures of hepatocytes, primary cultures and fetal brain cells, neuroblastoma cell lines, and the PC12 cell line.

Objective 4: Measurement of cell function under different aggregation conditions in gel culture. We have already developed methods of monitoring cell growth and metabolism in culture by measuring cellular protein, DNA, and lactate dehydrogenase (LDH) content. We have also developed methods for monitoring cell function in culture by following albumin and uric acid secretion (for hepatocytes) and expression of specific enzymes and responsiveness to nerve growth factor (for PC12 cells). Using the optimal experimental system, defined in specific objective 3, we will systematically examine the function of cell aggregates in culture. Aggregates will be cultured under a variety of conditions including i) conventional static culture, ii) static culture with aggregates suspended within gels of extracellular matrix molecules, and iii) microgravity culture of aggregates within the NASA rotating-wall bioreactors.

Objective 5: Preparation of experiments for evaluation under microgravity conditions. In Specific Objectives 1 through 4, we will have identified the important variables for controlling cell aggregation and function in aggregate culture. In the final stages of this project, we will design methods for developing physiologically realistic cell

aggregates under microgravity conditions and for testing the influence of aggregation on cell function in suspension culture under microgravity in space.

Task Significance:

These studies are uniquely suited for study in microgravity. First, cell aggregation in zero gravity will be driven by migration and diffusion rather than by forced collisions as is necessary on Earth. The resulting aggregates may be closer to those found in tissues since tissues are formed by migration and selective adhesion. Second, gentle suspension culture techniques can be used to culture the aggregates in microgravity. By the end of the period of laboratory study proposed here, we will have developed cell aggregation techniques appropriate for testing under microgravity conditions in space.

Progress During FY 1996:

Objective 1: We have synthesized several water-soluble molecules as molecular nuclei for cell adhesion. These molecules are based on poly(ethylene glycol) with bioactive peptides, $\text{NH}_2\text{-Gly-Arg-Gly-Asp (GRGD)}$ and $\text{NH}_2\text{-Gly-Tyr-Ile-Gly-Ser-Arg (GYIGSR)}$, grafted to the termini. We have developed covalent coupling methods for attaching these peptides to PEG with a variety of molecular weights (5,000 to 30,000) and to polystyrene microspheres (0.1 to 10 μm). We have used quantitative cell adhesion assays to determine the best peptides for conjugation. We have examined the kinetics of cell aggregation of a number of important cell types (including neural cells and cell lines, fibroblasts, and genetically engineered fibroblasts). We are developing methods for examining cell function for aggregates maintained in culture. The first report in this work was published this year (Dai, Belt, and Saltzman, 1994), and other publications are in progress.

Objective 2: We have synthesized polystyrene polymers modified with carbohydrates and peptides at the surface. A manuscript describing this work was published this year (Gutsche, et al., 1994). These unique, polystyrene-based polymers can be formed as microspheres, and cells attach and grow avidly to these novel microcarriers. We have developed similar methods for coupling peptides to polystyrene supports with a range of sizes.

Objectives 3 and 4: We have developed methods for culturing and forming aggregates under unit gravity. We have adapted these methods for producing aggregates within the NASA rotating-wall vessels. We have used aggregates of fibroblasts producing recombinant human NGF to demonstrate that aggregation under microgravity conditions increases the secretion rate of recombinant proteins (Dia and Saltzman, 1996).

Objective 5: This objective is only applicable to the third project year.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 11/92 EXPIRATION: 11/97
PROJECT IDENTIFICATION: 962-23-01-10
NASA CONTRACT NO.: NAG-654
RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

- Baldwin, S.P. and Saltzman, W.M. Polymers for tissue engineering. *Trends in Polymer Science*, 4, 177-182 (1996).
- Baldwin, S.P., Krewson, C.E., and Saltzman, W.M. PC12 cell aggregation and neurite growth in gels of collagen, laminin, and fibronectin. *International Journal of Developmental Neuroscience*, 14, 351-364 (1996).
- Dai, W. and Saltzman, W.M. Fibroblast aggregation by suspension with conjugates of poly(ethylene glycol) and RGD. *Biotechnology and Bioengineering*, 50, 349-356 (1996).
- Krewson, C.E. and Saltzman, W.M. Nerve growth factor delivery and cell aggregation enhance choline acetyltransferase activity after neural transplantation. *Tissue Engineering*, 2, 183-196 (1996).
- Mahoney, M.J. and Saltzman, W.M. Controlled release of proteins to tissue transplants for the treatment of neurodegenerative disorders. *Journal of Pharmaceutical Science*, (In Press).
- Saltzman, W.M. Growth factor delivery in tissue engineering. *MRS Bulletin*, (In Press).

Books/Chapters

Saltzman, W.M. "Cell Interactions with Polymers," in "Textbook of Tissue Engineering." Edited by: Lanza RP, Chick WL and Langer R (Ed.) Springer, NY, pp 227-248, 1996.

Robotic Acquisition and Cryogenic Preservation of Single Crystals of Macromolecules for X-Ray Diffraction

PRINCIPAL INVESTIGATOR: Dr. Craig D. Smith

University of Alabama, Birmingham

CO-INVESTIGATORS:

DeLucas, L.

University of Alabama at Birmingham (CMC)

Task Objective:

Experiments are aimed at the development of new or better methods of preserving protein crystals at ultra-low temperatures. Cryogenically preserved crystals can be used for immediate enhanced x-ray crystallographic data collection or stored indefinitely until data collection facilities become available.

Task Description:

The focus is on cryofluid/protein crystal interactions, thermal processes which affect the success of freezing protein crystals, and the development of rapid physical handling methods of these small fragile crystals to enhance success rates of cryofreezing. Understanding the freezing process on a molecular scale may provide more guidance to the current empirically derived methods.

Task Significance:

Protein crystals used for x-ray crystallographic experiments usually are very fragile and short-lived. Diffraction data from these crystals produce three-dimensional images of proteins important to many biochemical processes. Freezing protein crystals can greatly enhance the structural information obtained by crystallography by reducing their fragility and dramatically increasing their lifetimes. Experimental data also show that a clearer picture of the protein structure can result when the crystal is frozen.

Progress During FY 1996:

Significant progress has been made which has direct application to the planning of protein crystal growth and evaluation facilities for the International Space Station (ISS). A major overall goal has been to develop methods and tools for safely manipulating freezing and storing protein crystals. Understanding details and parameter limits of the crystal freezing process are vital to realistic design of procedures and apparatus.

Experiments were conducted to measure intensity decay rates for randomly selected reflections at various resolutions from thaumatin crystals at room temperature and frozen at 90 °K. The average decay rate for the unfrozen crystal is about twice that for the frozen crystal. Decay rates were calculated from linear slopes of intensity versus time graphs for the same set of reflections for a four day period.

It currently is unlikely that liquid nitrogen will be available on ISS for conventional methods of cryo-crystallography to be employed. Therefore a new method is required. Liquid oxygen is one attractive alternative we are considering. It is non-asphyxiating and containable by magnetic fields since it is paramagnetic. Conventional off-the-shelf cryogenic equipment (e.g., Oxford Cryostream) could be used with liquid oxygen with the addition of magnetic field containment in a supply dewar. Magnetic focusing of a low temperature gas stream onto the protein crystal is a useful idea for making low flow rates possible to conserve the liquid oxygen supply.

Experiments using the protein thaumatin have shown that useful high resolution data can be collected from frozen crystals up to 185 °K (-88 °C). These crystals were in typical growth buffer plus 20% glycerol. Data collection at this higher temperature would conserve the cryogenic gas supply or allow the use of conductive cooling an alternative freezing method under investigation. Conductive freezing was demonstrated in our lab using liquid nitrogen to cool a slender steel rod with a crystal mounting loop on the end. Experiments using a water cooled, three stage thermoelectric cooling device to conductive freeze similarly were not successful. The thermoelectric device from Melcor (Trenton, New Jersey) was not capable of removing enough heat at the required rate even when well insulated. A mechanical stifling cycle engine (Stirling Technology, Kennewick, Washington) however is capable of cooling at temperatures and wattages expected to be useful for keeping a protein crystal frozen to at least 185 °K and hopefully lower.

Thermal modeling and simulations of the freezing of liquids and crystals held in small loops have begun but are not completed. Sophisticated analytical calculations of loop freezing rates predict microsecond or faster freezing times. Experimental measurements of those times are being made. Fine electrode wires are used to measure resistance increase across the droplet during the course of freezing. The rapid change in resistance is monitored as a change in voltage drop across the droplet using a triggering memory oscilloscope. Preliminary results obtained by dipping the loop in liquid nitrogen indicate less than two milliseconds were required to freeze the droplet. This is much faster than the 1-2 seconds time measured by at least two other investigators using bulky epoxy coated thermocouples. This time scale also agrees with our theoretical calculations. Our results also indicate thawing times on the order of seconds. This means some time is available for transferring a crystal from a cryogenic freezer to another cryogenic location without active cooling for at least a few seconds.

A small inexpensive robotic arm has been purchased and assembled. It will be tested for transferring crystals accurately from one cryogenic location to another and doing it quickly enough to prevent thawing. Currently it appears feasible to use small loops for confident manipulation of protein crystals in growth liquids and for rapid through the air transfers. This idea will be tested in combination with the robotic arm. If proven this idea will greatly simplify the manipulation of protein crystals compared to current methods using fragile thin walled glass capillaries with suction.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 10/95 EXPIRATION: 10/96
PROJECT IDENTIFICATION: 962-23-08-47
NASA CONTRACT No.: NAG8-119
RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Smith, C.D. "Scenarios for handling Crystals Onboard Space Station." Macromolecular Crystallization Meeting, Panama City, Florida, April 29, 1996.

Influence of Microgravity Conditions on Gene Transfer Into Expanded Populations of Human Hematopoietic Stem Cells

PRINCIPAL INVESTIGATOR: Dr. F. M. Stewart

University of Massachusetts

CO-INVESTIGATORS:

Stein, J.
Lawrence, J.

University of Massachusetts Medical Center
University of Massachusetts Medical Center

Task Objective:

We plan to evaluate the ability of the High Aspect Rotating-Wall vessel (HARV) three-dimensional culture system to optimize engraftment conditions of human hematopoietic cells into SCID-NOD mice by evaluating a) its effects on purified stem cells and the development of stromal cells, b) cytokine stimulation in this system and expansion of stem cells, c) repetitive transplant, and d) cell cycle manipulation of stem cells. These conditions will set the stage for subsequent gene transfer studies with neomycin-resistance gene NEO^R transfection into primitive lymphohematopoietic stem cells.

Task Description:

We propose to use the HARV three-dimensional culture system and microgravity concepts to evaluate marrow cells from normal donors transduced with NEO^R, assessing long-term gene transduction frequency and gene expression, the effect of 5-FU pre-treatment (a method of cell cycling) on transduction frequencies in this system, and engraftment (with minimal or no myeloablation) into SCID-NOD animals. The results of these studies may show that the microgravity culture approaches may improve gene transfer, stem cell expansion, and engraftment into SCID-NOD animals. From these studies and others beyond the scope of this proposal, the potential benefits (and risks) of transferring other genes such as MDR1 into normal cells (or into cancer cells) may be assessed. Ultimately, as part of the future clinical gene therapy protocol, we plan to evaluate MDR1 gene transfer into normal marrow from patients with lymphoma in an effort to escalate doses with p 170 pump drugs such as Taxol, thereby potentially increasing cure rates while minimizing toxicity.

Task Significance:

Hematopoietic stem cells, because of their ability to repopulate bone marrow of myeloablated animals, have been an attractive vehicle for various gene therapy approaches. Work in different animal species and humans indicates an ability to transfer genes to hematopoietic stem cells using a variety of approaches including retroviral vectors. Genetically transduced hematopoietic stem cells have been transplanted into animals and humans, and the expression and long-term persistence of the genes has been demonstrated *in vivo*. Unfortunately, the level of expression and percent cells carrying the transferred gene have been disappointingly low in expression of the transferred gene, especially with progressive cell differentiation into different lineages. Alternate possibilities include a failure to transfer the gene of interest into long-term hematopoietic repopulating cells and/or a failure of these cells to engraft. Current culture systems are limited in supporting long-term preservation and expansion of stem cells. Since co-culture with gene-carrying viral supernatants appears at present to be the most effective method of gene insertion in human cells, optimizing culture conditions may be important for maximizing the efficiency of gene transfer into hematopoietic stem cells.

Progress During FY 1996:

We used the SCID-NOD animal model to assess growth characteristics of human cord blood cells and ultimately plan to assess *in vivo* transduction efficiencies of MDR1-transduced human bone marrow cells. We have performed over 21 experiments with cord blood and bone marrow injected into SCID-NOD animals. Unfortunately, in experiments conducted between April and July, and perhaps earlier, rotaviral and pinworm infections went unrecognized in our vivarium. Consequently, animals' deaths and failure to engraft human cells in these animals was noted. Avernectin, an antibiotic used to treat these infections, may have also contributed to engraftment failures. In selected experiments, we have achieved over 60% engraftment (CD45+) human cells. We have evaluated the effects of engraftment of radiation dose and fractionation, fractionation of cord blood, repetitive cell transplants, and mouse strain. Preliminary studies indicate that cells grown in HARV systems engraft in these

mice. Further studies evaluating new strains of mice that are radiation resistant and resistant to the development of thymic lymphomas that will permit more long-term assessment of stem cell growth are underway. Ultimately, once engraftment of human cells is optimized, we plan studies evaluating the growth of human bone marrow with or without *MDR1* gene transduction using the HARV system.

In other studies, we have substituted a Teflon ring designed by our engineering department for the plexiglass ring on the HARV system. We compared cell growth characteristics in HARVs using plexiglass rings (standard), Teflon rings, or Teflon bottle cultures. We have shown a 15% - 600% expansion of cell growth in vitro at 4 weeks with use of the Teflon ring over the other two approaches. We currently are analyzing the growth of CD34+ subpopulations and human HPP-CFC at two weeks in each of these systems. We plan to test 10 cc HARV systems to evaluate the growth of small numbers of CD34+ separated and unseparated populations of cells. Once culture conditions are optimized according to generation of CD34+ cells, we plan to explore co-culturing systems with human marrow cells in pVMDR1 retroviral vector supernatant (Ingenex) using the HARV system. We will evaluate retroviral gene transduction efficiency and the engraftability of these transduced cells into SCID-NOD animals.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/95 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 962-23-01-27

NASA CONTRACT No.: NAG

RESPONSIBLE CENTER: JSC

Mechanisms for Membrane Protein Crystallization: Analysis by Small Angle Neutron Scattering

PRINCIPAL INVESTIGATOR: Dr. David M. Tiede

Argonne National Laboratory (ANL)

CO-INVESTIGATORS:

Thiyagarajan, P.
Thurnauer, M.C.

Argonne National Laboratory (ANL)

Argonne National Laboratory (ANL)

Task Objective:

The goal of this project is to characterize structural intermediates in pathways for membrane protein crystallization. This project will use small angle neutron scattering, SANS, to characterize detergent and protein structures that exist in solution as a function of initial crystallization conditions, and this project will examine how these structures change as a function of time and trajectories that move the crystallization mixtures into metastable, crystallization phases.

Task Description:

This project will use the bacterial photosynthetic reaction center as a model for examining mechanisms for membrane protein crystallization, and for investigating the influence of the detergent on crystallization. Membrane protein crystallization differs from other protein processes by requiring the presence of a solubilizing detergent. The reaction center has been successfully crystallized in two types of detergent, zwitterionic lauryldimethylamine-N-oxide, LDAO, and non-ionic n-octyl-β-D-glucoside, OG. Conditions required for reaction center crystallization change depending upon the detergent used for solubilization of the reaction center. This demonstrates that the solubilities of both detergent and protein must be manipulated in order to successfully crystallize membrane proteins.

Protein crystallization is typically described in terms of three discrete phases: a solution phase where the detergent-solubilized protein complexes are soluble, a metastable crystallization phase where crystal nucleation and growth occur in the presence of solubilized protein, and finally a precipitation phase in which there is no solubilized protein in solution.

This project will use SANS to characterize how detergent and protein structures vary as a function of position in this phase diagram. Neutron scattering is sensitive to isotopic substitution. This project will use isotopic labeling to selectively extract neutron scattering contributions from the detergent and the reaction center structures in crystallization mixtures. These structures will be time-resolved during the time-course of crystallization.

Task Significance:

Protein crystallization is frequently a rate-limiting step in the analysis and understanding of the molecular basis for disease and drug therapy. This is particularly true for membrane proteins that are responsible for many major biological processes such as vision, nerve conduction, photosynthesis and respiration. So far there has been relatively little success in the crystallization of membrane proteins compared to water-soluble proteins. This project will provide unique, first-of-the-kind data on structural intermediates in pathways leading to the crystallization of the bacterial photosynthetic reaction center, which is one of the few membrane proteins that has been successfully crystallized. This information is necessary for the development of more general, rational strategies for enhancing the efficiency of membrane protein crystallization.

Progress During FY 1996:

A central issue concerning the mechanism of protein crystallization is determining whether protein aggregates serve as nucleation precursors or as the units for crystal growth. Determination of this feature is critical for developing rational strategies for protein crystallization. We have carried out neutron scattering measurements during the time-course of crystallization of the n-octyl-glucoside solubilized *Rhodobacter sphaeroides* R-26 reaction center using deuterated proteins, and with solution $^2\text{H}_2\text{O}/^1\text{H}_2\text{O}$ ratios that were contrast matched to that of the detergent. These conditions selectively enhanced scattering for the reaction center protein, while eliminating scattering from the detergent in the small angle domain. These measurements allowed us to selectively follow the solution structure of the reaction center during the crystallization time course without interference from detergent structures.

Small angle neutron scattering measurements taken during presaturation, nucleation, and crystal growth phases of crystallization revealed that the protein in solution remains in the monomeric state throughout this process. In the absence of a protein precipitant, the detergent solubilized reaction center was found to exist predominately in the monomeric form, although aggregated states were seen, accounting for 5% to 25% of the protein in different preparations. The addition of polyethylene glycol as the precipitating agent for crystallization at concentrations below the crystallization threshold caused rapid precipitation of the aggregated species. Guinier analysis of neutron scattering from the mixture showed that the reaction center protein at the start of a crystallization experiment is in a homogeneous, monomeric state, with undetectable amounts of aggregated species in the q range above $0.01 \text{ \AA}^{-1}$. Fitting of the scattering data with scattering calculated from reaction center crystal structures showed that less than 10% of the reaction centers exist in the form of dimers or other small aggregates. During crystal nucleation and growth, the solution state of the protein was found not to change. These findings indicate that a monodispersed reaction center-detergent particle is likely to serve as the precursor for this membrane protein crystal nucleation and to function as the crystal growth unit.

These results contrast markedly with analogous studies with water-soluble proteins. The absence of aggregation behavior for the detergent-solubilized reaction center is somewhat surprising, particularly in light of the micelle aggregation that occurs as consolution thresholds are approached. We noted in previous SANS studies that the presence of 10% PEG in OG micelle solutions eliminates salt induced aggregation of the micelles. It is possible that this mechanism is operating in the crystallization experiments described here. Current work is examining the role of the detergent in the crystallization process and is determining detergent structures during the crystallization time course.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/95 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 962-23-08-39

NASA CONTRACT NO.: H-13085D

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Books

Tiede, D.M., and Thiyagarajan, P. "Characterization of photosynthetic supramolecular assemblies using small angle neutron scattering (in "Biophysical Techniques in Photosynthesis")." Edited by: J. Ames and A.J. Hoff Kluwer Academic Publishers, Dordrecht, pp 375-390, 1996.

Tiede, D.M., Marone, P., Wagner, A.M., and Thiyagarajan, P. "Characterization of photosynthetic supramolecular assemblies using small angle neutron scattering (in "Photosynthesis: from light to biosphere")." Edited by: P. Mathis Kluwer Academic Publishers, Dordrecht, pp 431-436, 1995.

Preparation and Analysis of RNA Crystals

PRINCIPAL INVESTIGATOR: Dr. Paul Todd

University of Colorado, Boulder

CO-INVESTIGATORS:

Kundrot, C.E.

University of Colorado

Schultz, S.C.

University of Colorado

Task Objective:

Grow crystals of specific RNA's and nucleic-acid peptide complexes that diffract x-rays to high resolution.

Identify pathways that lead to highest-quality crystals of RNA's and complexes.

Detail the mechanism of the role of inertial acceleration (gravity) in high-resolution RNA crystal growth.

Task Description:

1. Preparation of high-quality crystals and their complexes.
2. Pathway to high-quality RNA crystals.
3. Mechanism of action of inertial acceleration (gravity) on crystal growth.

Task Significance:

There is a rising interest in the use of specially-tailored RNA sequences as pharmaceutical and diagnostic chemicals. These sequences must have a three-dimensional structure that allows them to interact with target molecules, usually proteins. One example is a 28-base RNA sequence that inhibits the reverse transcriptase of HIV-1; this target molecule is required for the replication of the AIDS virus in human cells. Another is a longer RNA that behaves like an enzyme and enzymatically cleaves virus RNA in cells. To assess the ability of these RNA's to interact with their targets and to possess chemical stability, their three-dimensional structure needs to be determined by x-ray crystallography, which requires high-quality crystals at least 0.5 mm long. However, there is very little experience, worldwide, in crystallizing RNA's. Therefore the goals of this project are to provide high-quality RNA crystals and a paradigm for their reliable preparation.

Progress During FY 1996:

1. Preparation of high-quality crystals of RNA's and their complexes: Using hanging-drop, sitting-drop and osmotic dewatering methods, diffraction-quality crystals of the oligonucleotide "UU-dodecamer" were grown to 0.3 mm or more in length. Two growth habits were noted for crystals having the same space group. Average resolution was better than 3.0 Å and maximum resolution was 2.46 Å by all crystallization methods. The structure of this molecule was solved and published. A second oligonucleotide, a 35-base Nexamer molecule "225T3," which reacts with insulin-like growth factor has been chosen as the next example to crystallize. Initial screens have been completed and refinements are underway using hanging-drop, osmotic dewatering and low-gravity techniques. Samples are being prepared for space shuttle mission STS-80 using "C-MIX" payload hardware.
2. Pathway to high-quality RNA crystals: A controlled dewatering device has been tested and modeled. The rate of water removal through a reverse osmosis membrane has been analyzed in complete detail by a model equation in closed form that requires only one fitted parameter, the Darcy's-law membrane resistance, R_m . The theory has been successfully tested on a multichamber osmotic dewatering device capable of crystallizing 24 samples simultaneously, enough for a sparse-matrix screen using this method. Furthermore, by controlling the osmolarity drop across the membrane, a dewatering profile identical to that achieved by vapor diffusion (hanging drop) has been achieved, and UU-dodecamer crystals grown by both methods at the same rate are of comparable quality. The role of the control achieved by the osmotic dewatering method was further confirmed by dynamically adjusting the dewatering rate to allow (1) early nucleation at high saturation rate followed by (2) a period of quiescent growth at lower saturation and finally (3) continued growth by return to higher saturation after initial equilibrium was

achieved. The resulting crystals were the product of more highly controlled nucleation and growth to larger final size. The effect of purity has also been tested in three ways: (1) crystal growth in samples of 89% vs. 95% purity have been compared with a small increment in crystal size and quality at the higher purity; (2) the growth of crystals in deliberate mixtures of UU-dodecamer and a closely-related derivative of the same size with smaller and lower-quality crystals appearing in the presence of increasing concentrations of the derivative; and, (3) ion-exchange chromatography has been found to rival gel electrophoresis for oligonucleotide purification.

3. Mechanisms of action of inertial acceleration (gravity) on crystal growth: the highest-quality crystal grown by osmotic dewatering was produced in a space-hardware version of the crystallizer; however, this crystallizer, "Fluid Processing Apparatus (FPA) Insert," is subject to erratic behavior that appears to be due to a combination of membrane variability and method of assembly. This device has been further characterized in preparation for continued low-gravity crystallization experiments. The UU-dodecamer normally crystallizes at 37 °C and has not been observed to form crystals at lower temperatures; however, in one low-gravity experiment performed at 23 °C a small crystal was seen to form. Using hen-egg lysozyme as surrogate in ambient-temperature studies in low gravity, the concepts developed in part 2, above, were tested by changing osmotic gradients during flight and during crystal growth. The expected outcomes were observed; namely, larger, more regular, protein crystals. This concept is now ready for testing in forthcoming low-gravity experiments with oligonucleotides.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 2
MS Students: 1
PhD Students: 1

TASK INITIATION: 9/95 EXPIRATION: 7/96

PROJECT IDENTIFICATION: 962-23-08-42

NASA CONTRACT NO.: NAG8-116

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Lietzke, S.E., Barnes, C.L., Berglund, J.A., and Kundrot, C.E. The structure of an RNA dodecamer shows how tandem U-U base pairs increase the range of stable RNA structures and the diversity of recognition sites. *Structure*, vol. 4, 917-930 (1996).

Sygusch, J., Coulomb, R., Cassanto, J.M., Sportiello, M.G., and Todd, P. Protein crystallization in low gravity using a novel liquid-liquid diffusion method. *J. Crystal Growth*, vol. 162, 167-172 (1996).

Proceedings

Cassanto, J.M., Morrison, D.R., Hymer, W., Todd, P., Korszun, Z.R., Mosier, B., Edmundson, A., Sygusch, J., Bower, D., Kearney, G.P., Dunfee, W., Alvarado, U., Guintini, R., and Bem, M. "Concept of a commercial automated biotechnology space processing payload onboard the space shuttle and space station." *Proceedings of the Space Technology & Applications International Forum*, Albuquerque, New Mexico, Institute for Space Power, University of New Mexico, June 2-3, 1996.

Johnson, T., Todd, P., and Stodieck, L. "Microgravity: New opportunities to facilitate biotechnology development." *Proceedings of the Space Technology & Applications International Forum*, Albuquerque, New Mexico, Institute for Space Power, University of New Mexico, paper #275, 1996.

Lee, C.Y., Sportiello, M.G., Cape, S., Ferree, S., Todd, P., Kundrot, C.E., and Barnes, C. "Application of osmotic dewatering to the crystallization of oligonucleotides for crystallography." *Proceedings of 25th Biochemical Engineering Symposium*, R. Bajpai, ed., University of Missouri, Columbia, Missouri, 1995.

Sportiello, M.G., Todd, P., Lee, C.-Y., Kundrot, C.E., Schultz, S., Stodieck, L.S., and Cassanto, J.M. "High frequency access to low gravity experimentation in organic crystal growth from solutions." *Proc. Space 96, 5th International Conference on Engineering, Construction and Operations in Space*, Albuquerque, New Mexico, June 2-6, 1996.

Presentations

Cape, S.P., Lee, C.-Y., Petrini, K., Ferree, S., Sportiello, M.G., and Todd, P. "Chromatographic purification of oligonucleotides: comparison with electrophoresis." *Colorado Biotechnology Symposium*, Ft. Collins, Colorado, 1996.

Cape, S.P., Lee, C.-Y., Petrini, K., Ferree, S., Sportiello, M.G., and Todd, P. "Chromatographic purification of oligonucleotides: comparison with electrophoresis." *Biochemical Engineering Symposium*, Manhattan, Kansas, 1996.

II. MSAD Program Tasks — Ground-based Research

Lee, C.-Y., and Todd, P. "Characterization and application of osmotic dewatering to the crystallization of biomolecules." American Chemical Society Annual National Meeting, New Orleans, Louisiana, March 24-28, 1996.

Lee, C.-Y., Sportiello, M.G., Cape, S.P., Ferree, S., Todd, P., Kundrot, C.E., Lietzke, S., and Barnes, C. "Characterization and application of osmotic dewatering to the crystallization of oligonucleotides." Colorado Biotechnology Symposium, Ft. Collins, Colorado, 1996.

Lee, C.-Y., Sportiello, M.G., Cape, S.P., Ferree, S., Todd, P., Kundrot, C.E., Lietzke, S., and Barnes, C. "Characterization and application of osmotic dewatering to the crystallization of oligonucleotides." Biochemical Engineering Symposium, Manhattan, Kansas, 1996.

Todd, P. "Analysis of crystallization by osmotic dewatering and its application to oligonucleotides." Protein Crystal Growth Conference, Panama City Beach, Florida, April 28-30, 1996.

Development of Microflow Biochemical Sensors for Space Biotechnology

PRINCIPAL INVESTIGATOR: Dr. Bruce Towle

Arizona State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The overall objective of this work is to develop an approach to biochemical concentration sensing that can accurately track glucose and oxygen concentrations in bioreactor media over several week durations and operate successfully in a space environment. Our approach to this problem has been the development of sensor systems which use minute quantities of reagents that change color in response to chemical concentration. In some respects, these systems are basically miniature versions of benchtop flow injection analyzers for glucose and oxygen, but scaled down in size and made more robust and suitable for continuous on-line monitoring of bioreactors. The output of these sensors will potentially allow feedback control of nutrient concentration in cell culture in order to maintain a more constant cell growth environment than can be achieved without sensors.

During this first year of the project, we have focused on the development of hardware and the evaluation of reagent systems for a chemical stability and suitability for the requirements of space bioreactors. In this coming year, we anticipate the development of systems that will mimic space bioreactor operation, which will allow us to adequately test the sensors for long-term stability.

Specifically the project objectives are:

1. To test microdialysis methods as a means of reliable sample withdrawal from the bioreactors.
2. To develop more optimal techniques for the improved storage of the sensor reagents without refrigeration.
3. To identify ways to fabricate the sensors in a reliable and maintenance free configuration.
4. To develop a testing protocol that conforms to the operating conditions the sensor will experience in space bioreactors. This will allow final shakedown and identification of possible problems with final sensor integration into the configuration used for flight.

Task Description:

The project consists of developing the principles and manufacturing approaches of a microflow biochemical analysis system for application to space bioreactors. A microflow colorimetric sensor for glucose is being constructed based on the use of a predissolved single reagent system. The Signa Inc., (St Louis, Mo.) "Trinder test" employs peroxidase and glucose oxidase enzymes with another dissolved reagent to produce, in the presence of glucose, stoichiometric amounts of a colored dye that is measured photometrically.

The basic glucose sensing strategy is to pump submicroliter quantities of Trinder reagent and a dialyzed sample of filtered bioreactor media into a common mixing plenum. The project partially concerns the development of a fluid handling system that is resistant to bubble formation or other problems brought on by the forces of liftoff, pressure and temperature changes, and zero gravity operation.

The space bioreactor hardware implementation of a fluorescent oxygen sensor under development uses an oxygen-sensitive fluorescent dye trapped in a micro-flow recirculating loop. The system employs a length of gas-permeable thin silicone tubing that is immersed in the bioreactor solution or media flow loop as a way of sampling oxygen concentration. The portion of the flow exiting from the bioreactor media is immediately subjected to a fluorescence test by an in-line optical cell. The dye is then recirculated back to a small, several-milliliter holding reservoir for reuse.

The important problems and issues under research are the best way to implement the microflow system so that it resists bubble formation, effects of zero gravity, and methods to allow the system to self-check and recalibrate itself periodically. We are also trying to determine ways to minimize the amounts of reagents that can be used in the system for two-week to one-month missions in order to make the sensor compact. Research is being conducted to

II. MSAD Program Tasks — Ground-based Research

find ways to improve the shelf life of reagents, which is currently a limiting factor, so that we can achieve sensor operational lifetimes of more than one month.

Task Significance:

Maintenance of cell culture environments in terms of pH, glucose, and oxygen tension is of particular importance to the successful growth of mammalian cells. Variations in these quantities, which can easily occur with rapid cell growth, can be confounding variables in interpretation of results obtained from cell cultures grown in space. Additionally, the range of permissible biochemical variation in culture media is narrow and specific to a given cell type. For this reason, a critical requirement of successful space bioreactor operation is the measurement of the concentration of biochemicals in cell growth media. This information would then be used by a control system to maintain cell culture chemical balances. Unfortunately, the rigorous demands placed on biochemical sensors by space biotechnology reactors precludes the use of commercially available biochemical sensors that meet the size, weight and bulk requirements of flying in a space shuttle locker. As a result, a good argument could be made that lack of suitable biosensors is one of the primary factors presently limiting the success of biotechnology reactors in space.

Progress During FY 1996:

Research over the past year suggests that our microflow-colorimetric biochemical sensor approach continues to look promising for biotechnology applications in space. Cell culture carbon dioxide sensors suitable for long-term immersion in bioreactors and constructed using the same basic design approach as our microflow glucose, oxygen, and pH sensors have performed excellently over nine-day durations in circulating-flow test environments. The test showed a stability to better than ± 2 mm-Hg at 37°C as compared to a benchtop Radiometer gas analyzer used as a standard.

The improved design of a microflow oxygen sensor uses very fine microbore silicone tubing that interfaces to a sensor-block that is placed in series with a bioreactor flow loop. The microflow-fluorescent cell culture oxygen sensor continues to show outstanding long-term stability using a RTDP colorimetric reagent while its temperature sensitivity is being addressed using software compensation.

We have changed the original design strategy of using segmented flow streams to that of continuous microflow systems. This has simplified the hardware and so improved the expected reliability and maintainability. Problems of sensitivity to bubble formation in the sensor have been effectively eliminated by using water-insoluble gasses rather than air as propellants to the reagent flow stream.

The progressive development of the hardware has entailed the evaluation of several different approaches to microflow reagent delivery to the sensor chemistry block. The most recent and so far most successful system has been the use of pressurized reagent reservoirs employing lengths of resistance capillary tubing as the flow regulation element. This approach has successfully produced a sensor system that employs a one micrometer per minute flow rate of reagent. This results in the consumption of relatively small amounts of reagent, about 20 milliliters over a two-week duration. We are currently working on an improved system that uses microvalves that will extend this quantity of reagent up to several months.

Two different microflow glucose sensor configurations and hardware implementations have evolved out of our research, one using a glucose oxidase-based test (Trinder test) and another using a nonenzyme test (Toluidine test). The lifetime of the glucose sensor Trinder reagents have been a limiting factor in its long-term performance. This problem seems largely solved by modifying the reagent's chemical composition, primarily by increasing the concentration of the oxidase enzymatic components. This has resulted in usable performance of the reagent over a one-month duration. The Toluidine-based reagent and sensor system for glucose has a potentially indefinite lifetime. Tests of the electronics and optical cell subsystems indicate that an operational stability of at least $\pm 5\%$ accuracy can be achieved. However, this sensor has certain tradeoffs to obtain longevity in terms of a more complex hardware implementation and a lesser glucose specificity since it is also substantially responsive to galactose, which unfortunately may restrict its use to certain kinds of cell culture media.

The integral sensor microcontroller system allows self-testing and automated operation of the sensor. We are currently looking at implementing a strategy to use software programming to recognize measurement artifacts due to the presence of gas bubbles in the bioreactor flow streams. These kinds of artifacts have been shown in past shuttle flights to be a particular problem with bioreactors operating in zero gravity.

Despite several design modifications and improvements, the overall sensor system for oxygen and glucose continues to be relatively compact and occupies approximately 800 cc of total volume including reagents sufficient for a two-week bioreactor mission. Its power demands have also been kept minimal, to less than a few watts.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-23-01-33

NASA CONTRACT No.: NAG9-815

RESPONSIBLE CENTER: JSC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Cooney, C. and Towe, B.C. Carbon Dioxide Measurement by Microflow Colorimeter. Journal of Biosensors and Bioelectronics, (In Press).

*Experimental Studies of Protein Crystal Growth Under Simulated Low-Gravity Conditions***PRINCIPAL INVESTIGATOR:** Dr. Eugene H. Trinh

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:DeLucas, L.J.
Rhim, W.K.University of Alabama, Birmingham (UAB)
Jet Propulsion Laboratory (JPL)**Task Objective:**

The goal of this ground-based experimental research task is to better establish the role of convective flows in the determination of the characteristics of crystals grown from protein solutions. The primary objectives are first to inhibit natural convective flows around isolated crystals immersed in single levitated solution droplets, and then to either allow natural convection to occur or to carefully increase the magnitude of an artificially-induced convective flow. The secondary objective is to develop a new experimental approach for the detailed characterization of the crystal environment while providing simulated low gravity conditions in 1-g by using freely levitated solution droplets rotating along a horizontal axis.

Task Description:

A specific objective is to obtain a quantitative measure of the effects of varying the flow velocity around a crystal by at least one order of magnitude while maintaining all the other relevant parameters constant. The specific tasks are to measure the face growth rate and to monitor the depletion layer around a growing crystal while inhibiting convection. We will first attempt to visualize it in the simulated low-gravity condition, and then perturb it by the induction of controlled flow fields. The flows within the levitated solution drops will be monitored by elastic light scattering methods, while the evolution of the protein aggregates will be examined through nonelastic dynamic light scattering and Raman spectroscopy.

Task Significance:

The influence of gravitational effects on the evolution of living and inorganic crystalline materials has been recently underscored by investigations performed in microgravity. In particular, strong circumstantial evidence has been gathered pointing to the marked improvement in the characteristics of protein crystals grown in low Earth orbit. The importance of understanding the structure of the assembly of proteins molecules for application to the biotechnology and pharmaceutical fields makes the identification of the specific gravity-related processes of particular significance. Understanding and perhaps eventually controlling the right parameters on Earth will significantly impact our ability to improve our methods to grow proteins in order to extract more valuable information to be used for the manufacture of drugs and to better understand biochemical processes affecting human health.

Progress During FY 1996:

A new ultrasonic-electrostatic droplet levitation apparatus has been assembled and implemented in the ground-based investigation of the rotational control capabilities. We have demonstrated that slow (0.5 rps) as well as relatively fast (3-5 rps) rotation along a horizontal axis can be imparted to an electrostatically levitated droplet of 3-4 mm in diameter. We have also experimentally verified the correlation between the ultrasonic streaming flow patterns in the air surrounding the levitated drop and the rotational motion of the droplet.

The currently available capabilities of the experimental apparatus includes:

- Automated droplet size measurement through both electric field measurement as well as digital video image analysis of the magnified image of the levitated drop.
- Humidity control of the levitation chamber which allows a programmed decrease of the levitated droplet size. The capability of maintaining the droplet volume constant Over a long period of time (1 hour) has been verified, and preliminary success in increasing the droplet size has also been obtained.

Additional capabilities under current development include:

- Droplet temperature control using a thermally isolated chamber capable of maintaining the surrounding gas temperature at 4 °C and pulsed low-power laser heating of a rotating or stationary droplet for rapid temperature changes.
- Small probe for the measurement of the pH of the solution droplet.
- Raman scattering from the levitated solution droplets using CCD array detectors for real time monitoring of the solution composition.
- Dynamic light scattering from the levitated solution droplets in order to obtain information on the nucleation dynamics within the solution.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 11/95 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 962-23-08-40

NASA CONTRACT NO.: no #

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Chung, S.K., and Trinh, E.H. "An ultrasonic-electrostatic hybrid levitator for crystal growth from solution." Joint Acoustical Societies of America and of Japan (abstract accepted), December 2-6, 1996.

Trinh, E.H. "Development of a Rotating Levitated Drop Apparatus for Crystal Growth from Solution." 1996 Protein Crystal Growth Conference, Panama Beach City, Florida, April 28-30, 1996.

Two-Dimensional Protein Crystallization at Interfaces

PRINCIPAL INVESTIGATOR: Dr. Viola Vogel

University of Washington

CO-INVESTIGATORS:

Stayton, P.

University of Washington

Task Objective:

The primary objective of our program is to develop extensive insight into the biophysical chemistry of protein crystallization, with simultaneous emphasis on developing new approaches for catalyzing three-dimensional protein crystal growth. Genetic engineering techniques and powerful *in situ* optical imaging and spectroscopy methodologies will be used to dissect the biomolecular structure-function relationships governing crystallization. The site-directed mutagenesis of streptavidin will allow the mapping of specific protein side-chains to specific physico-chemical roles in crystallization. These physico-chemical roles will be experimentally elucidated using an array of cutting-edge surface analytical techniques.

Task Description:

Our first two tasks are (1) to study the effects of reduced biotin-binding affinity on the two-dimensional crystallization process by the use of site-directed streptavidin mutants, and (2) to characterize how site-directed side-chain alterations of the *lateral* protein-protein contact zones affect two-dimensional crystallization (i.e., crystal growth, size, and morphology).

Modern *in situ* surface analytical techniques will be employed and further developed to probe (a) the surface binding of the model protein, (b) the two-dimensional crystallization processes, and (c) the growth rates. The surface binding, as well as the size and shapes of resulting crystals, will be characterized as a function of the binding affinity to the surface anchored ligands. The crystallization of streptavidin underneath biotinylated surfaces will serve as our first model system.

Task Significance:

Despite the importance of protein crystallization to many fields in the biological sciences, the biotechnology field, and the pharmaceutical industry, there remains a striking paucity of fundamental principles describing protein crystal nucleation and growth. Our program is aimed at filling this gap, by providing molecular insight into the biomolecular structure-function relationships governing protein crystallization in the model streptavidin two-dimensional system that is amenable to *in situ* physico-chemical characterization. Site-directed mutagenesis experiments allow us to alter selected protein side-chains. We will probe the resulting changes in physical parameters of the crystallization process as a function of these changes using a combination of surface analytical techniques.

In situ monitoring of crystallization processes is an important need for microgravity environment research, as very little information is available for how the dynamics compare to ground-based growth. Thus, although our first generation of proposed experiments are designed for ground-based research, the optical and mass sensitive techniques to be utilized in these experiments should be readily adapted to future in-space applications.

Progress During FY 1996:

We have accomplished major progress in several of the following key areas:

Development of Brewster angle microscopy (BAM) as a quantitative probe to measure the protein surface density at surfaces under in situ conditions:

The two-dimensional crystallization of proteins is induced by attracting proteins to interfaces, for example, via high affinity binding to surface bound ligands. The advantage is that the individual proteins all attain similar orientation upon surface binding, and that supersaturated protein concentrations can be reached at the interface even at moderately low protein bulk concentrations. We have shown that the protein surface densities can be probed quantitatively by BAM. This is of significance as the quantitative analysis of the gray scale of BAM images sheds

light into the nature of the non-crystalline-to-crystalline phase transition of proteins. We found that the crystallization of our model protein streptavidin underneath functionalized lipid monolayers follows a first-order phase transition. The density of streptavidin bound to a biotinylated monolayer has to reach 75% of the crystalline density before a 2-D crystallization is induced. This critical surface density is remarkably high. In agreement with the basic thermodynamic theory, the critical surface density is independent of the protein concentration in the bulk solution. These experiments required the derivation of a quantitative relationship between BAM-image gray scales and protein surface coverage.

Development of alternative methods to bind and orient proteins at interfaces:

Several methods are currently under investigation to orient proteins at interfaces. However, only a few have been used successfully for the 2-D crystallization of proteins. We were able to show that the naturally occurring surface histidines of streptavidin can be utilized to bind streptavidin to a metal chelating surface monolayer, and to induce its 2-D crystallization. Our goal is to show that this approach is general and can be applied to proteins that may not have high affinity ligand binding sites. It should be noted that the shape of the 2-D streptavidin crystals, as well as the critical surface density for crystallization, are significantly different for streptavidin bound to the surface via high affinity ligand binding, or bound via surface histidine coordination to a copper-bound metal chelator.

Protein-protein molecular recognition in crystal formation:

Protein-protein molecular recognition underlies protein crystallization processes, but very little is known of the relationships between specific hydrogen bond, salt-bridge, and van der Waals' interactions and crystallization properties. We have used site-directed mutagenesis techniques to selectively alter the C-terminus of streptavidin which is involved in forming the protein-protein contacts in the two-dimensional crystals. These studies, along with further mutagenesis work of hydrogen bonding and salt-bridge contacts, are beginning to define the important contacts which provide the energetic basis for protein crystallization.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 9/95 EXPIRATION: 8/99
PROJECT IDENTIFICATION: 962-23-08-45
NASA CONTRACT NO.: NAG8-114
RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Frey, W., Schief, Jr., W.R., and Vogel, V. Two-dimensional crystallization of streptavidin studied by quantitative Brewster Angle Microscopy. *Langmuir*, vol. 12, 1312-1320 (1996).

Frey, W., Schief, Jr., W.R., Pack, D., Chen, C.-T., Chilcote, A., Stayton, P.S., Vogel, V., and Arnold, F.H. 2-D protein crystallization via metal-ion coordination by naturally-occurring surface histidines. *Proc. Natl. Acad. Sciences USA*, vol. 93, 4937-4941 (1996).

Presentations

Stayton, P. "Proteins at Interfaces." University of Wisconsin, November 1995.

Stayton, P. "Engineering molecular recognition events at biomaterial interfaces." Naval Research Laboratory Workshop on Non-Biomedical Applications of Biomaterials, August 1996.

Stayton, P. "Molecular recognition in the streptavidin-biotin system." Georgetown University, April 1996.

Stayton, P. "Proteins at Interfaces." Biorecognition at Interfaces Symposium at the 70th Colloid and Surface Science Symposium, American Chemical Society, June 1996.

Stayton, P. "Proteins at Interfaces." Duke University, April 1996.

Vogel, V. "Two-dimensional protein crystallization at interfaces." Max-Planck Institute for Polymer Research, Mainz, Germany, July 1996.

II. MSAD Program Tasks — Ground-based Research

Vogel, V. "Two-dimensional protein crystallization at interfaces." Technische Universität, München, Germany, July 1996.

Vogel, V. "Surface recognition to orient, crystallize and direct the motility of proteins at interfaces." Gordon Conference on Biomolecular Recognition and Immobilization, August 1996.

Vogel, V. "2-D protein crystals." Summer School of the Laboratory for Exotic Nanomaterials, Riken Frontier Research Institute, Wako, Japan, August 1996.

Vogel, V. "Langmuir monolayers as model for the study of early nucleation events." Workshop on Molecular Engineering of Inorganic Materials at Organic Interfaces, Friday Harbor, Washington, September 1996.

Vogel, V., Frey, W., Schief, Jr., W.R., and Stayton, P.S. "Critical surface density and protein/protein contacts in 2-D protein crystallization." Protein Crystallization Conference, Panama City Beach, Florida, April 1996.

Vogel, V., Frey, W., Schief, Jr., W.R., Chilkoti, A., and Stayton, P.S. "Dynamics of Protein Aggregation and Crystallization at Interfaces." MRS Meeting, Boston, Massachusetts, November 27 - December 1, 1995.

Automation of Protein Crystallization Experiments: Crystallization by Dynamic Control of Temperature

PRINCIPAL INVESTIGATOR: Dr. Keith B. Ward

Naval Research Laboratory (NRL)

CO-INVESTIGATORS:

Zuk, W.M.

Geo-Centers, Inc./Naval Research Laboratory (NRL)

Perozzo, M.A.

Naval Research Laboratory (NRL)

Task Objective:

The goal of this research program is to develop a dynamically-controlled crystallization system (DCCS) in which protein supersaturation is controlled by varying the temperature while crystallization is monitored by optical means. This device will also be capable of being controlled telerobotically. The program intends to extend its accomplishments in this area by continuing to enhance the DCCS, expanding the system to include multiple crystallization chambers and incorporating more efficient and versatile systems for monitoring the progress of nucleation and crystallization. A final goal of this project is to ascertain to what extent the technique of temperature-controlled crystallization is applicable for protein crystallization.

Task Description:

A study of a representative sample of well-characterized proteins that have been successfully crystallized using other methods is proposed. The temperature coefficient of solubility will be measured using the DCCS, and attempts to prepare crystals in this apparatus will allow us to judge the general usefulness of this approach. The proposed methods of research include incorporating dynamic light scattering to monitor the onset of protein nucleation. Telerobotic control experiments will continue using enhanced control software, and the results of the experiments will be aimed at defining the capabilities and limitations of remotely-controlled crystallization protocols on space platforms in microgravity. Collection of protein temperature solubility data will be enhanced by the development of more fully automated software algorithms. The temperature of a sample is slowly changed step-wise until the level of scintillation signal indicates that the crystallization phase boundary has been crossed. The temperature will then be recycled using a finer step size until the solubility temperature of the sample is determined to within 0.1 °C. Although currently some of this process is conducted manually, further development of the control software will completely automate the process.

Task Significance:

This research is important in continuing the development of dynamically-controlled crystallization systems, proving the usefulness of dynamic control in conducting protein crystallization experiments in microgravity. This work will also aid the current effort of other NASA-funded Principle Investigators in designing advanced crystallization apparatuses. This system will also be used, while it is being developed, to explore whether temperature control of supersaturation is a technique that can have wide applicability in laboratory-based protein crystallization.

Progress During FY 1996:

The miniaturized dynamically controlled temperature device has been used to collect preliminary solubility data on hen egg-white lysozyme, α -chymotrypsin, ferritin, ribonuclease A, and catalase. Some success was achieved in crystallizing lysozyme and ferritin through temperature control. The control software which operates the crystallization device is being redesigned to permit simultaneous multiple experiments and to enhance the analysis of intensity data. We have also initiated the integration of dynamic light scattering equipment into the apparatus to study the effects of temperature on protein aggregation.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 1/93 EXPIRATION: 1/96

PROJECT IDENTIFICATION: 962-23-08-24

NASA CONTRACT NO.: H-07975D

RESPONSIBLE CENTER: MSFC

Thermal Optimization of Growth and Quality of Protein Crystals

PRINCIPAL INVESTIGATOR: Dr. John M. Wiencek

University of Iowa

CO-INVESTIGATORS:

Rutgers University

Arnold, E.

Task Objective:

The overall goal of this project is to control supersaturation at constant values during protein crystal growth by varying the temperature in a predetermined (by simple theory) manner. Applying the theory requires knowledge about specific physico-chemical properties of the protein solution including the effect of supersaturation on growth rates and the effect of temperature on protein solubility. Our specific goals are:

- Application of a temperature control strategy (which maintains constant supersaturation) to the growth of lysozyme crystals and comparison to traditional isothermal strategies.
- Investigation of batch isothermal calorimetry as a tool to determine lysozyme solubility as a function of temperature by employing the Van't Hoff equation.
- Construction of a video microscopy apparatus for determination of crystal growth rates and terminal size.

Work for the coming year will focus on the measurement of solubility and crystal growth rate for catalase and thaumatin as well as the assessment of the crystals grown by the developed strategies via x-ray diffraction.

Task Description:

Four protein systems have been chosen for study: lysozyme, catalase, thaumatin and HIV reverse transcriptase. Each of these proteins have unique features that make them interesting. Lysozyme, catalase, and thaumatin represent fairly inexpensive and readily available proteins and will be model systems for investigations elucidating the effects of growth rates on crystal quality. Once strategies that are optimal are available, such strategies will be applied to the RT system as a realistic test case.

Experimental evidence suggests that larger and higher quality crystals can be attained in the microgravity environment of space. Fundamental studies have attempted to measure and model the effects of gravity-induced convection and sedimentation on the crystal growth process. However, the effect of growth rate on protein crystal quality is not well documented. If the growth rate is controlled, how much time is required to allow for interfacial attachment of the large protein molecule? What is the impact of this "attachment time" on crystal quality? This research effort is directed at measuring the effects of crystal growth rate on the ability of crystals to diffract x-rays. We hope to link crystal quality to slow growth rates and discern "how slow is slow enough." In addition, processing strategies will be developed which x-ray crystallographers can use to grow larger, high-quality crystals. The investigation requires the measurement of protein (lysozyme, catalase, thaumatin and RT) solubility at two or more different temperatures (typically 4 ° and 25 °C) and the growth rate at two or more different supersaturations. Microcalorimetry is a potentially powerful technique to measure these and other (e.g., nucleation) physical parameters of the protein systems.

Task Significance:

Development of a systematic method of protein crystallization may lead to crystallization of previously uncrystallizable proteins and add to current knowledge of protein structure/function relationships. Knowledge of detailed protein structure is essential for rational design of therapies and small molecule pharmaceuticals.

Progress During FY 1996:

Work is progressing on the use of predictive temperature control algorithms to maximize crystal size and quality. Our previous efforts have shown that the predictive temperature profiles for lysozyme can lead to fewer, larger crystals with notable improvement in crystal quality. Current efforts have focused on the extension to other protein systems. The physico-chemical parameters required to implement such temperature profiles include the heat of crystallization, growth rate functionality in terms of supersaturation, and the location of the labile zone. We are deriving theoretical as well as practical methodologies based on microcalorimetric measurements to obtain such

information. The results to date with lysozyme have proven our theoretical expressions correct provided care is taken when determining terminal crystal sizes. Using these parameters, we are concurrently growing crystals of Thaumatin via our temperature control algorithm. Work for the next year will continue along these lines.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	4	PhD Degrees:	1

TASK INITIATION: 6/93 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-23-08-28

NASA CONTRACT NO.: NAG8-115

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Schall, C., Arnold, E., and Wiencek, J.M. Enthalpy of Crystallization of Hen Egg White Lysozyme. *J. Cryst. Growth*, vol. 165, 293 (1996).

Schall, C., Bonita, J., Li, E., Arnold, E., and Wiencek, J.M. Application of temperature control strategies to the growth of hen egg-white lysozyme crystals. *J. Cryst. Growth*, vol. 165, 299 (1996).

Presentations

Bonita, J., Arnold, E., and Wiencek, J.M. "Effect of Crystal Growth Rate on Protein Crystal Quality." AICHE Annual Meeting, Miami Beach, Florida, November 1995.

Darcy, P.A., and Wiencek, J.M. "Thermal Analysis of Protein Crystallization." Symposia on Protein Crystallization, American Chemical Society Meeting, New Orleans, Louisiana, March 24, 1996.

Wiencek, J.M. "Protein Crystallization: Microcalorimetric Investigations & Thermally Controlled Growth." NASA Protein Crystal Growth Conference, Panama City Beach, Florida, April 1996.

Wiencek, J.M. "Effect of DMSO on Peroxidase-Catalyzed Polymerization of Cresol." U.S. Army Edgewood Research, Development, and Engineering Center Scientific Conference on Chemical Defense Research, November 15, 1995.

Search for a Dilute Solution Property to Predict Protein Crystallization

PRINCIPAL INVESTIGATOR: Dr. W. W. Wilson

Mississippi State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The primary objective of this research is to discover a unique dilute solution parameter that universally and unambiguously predicts protein crystallization.

Since most crystallographers will not have access to sophisticated laser scattering instrumentation, a secondary objective of this research is to construct a simple laser scattering device that determines the universal predictor values. The device will be miniaturized to work with sub-milliliter volumes and incorporate the latest optical fiber technology for beam delivery and signal detection and for temperature control.

Task Description:

Static, dynamic and electrophoretic laser scattering techniques will be used to carefully measure an array of thermodynamic and hydrodynamic (not kinetic) solution parameters for each of a group of selected proteins dissolved under crystallizing as well as non-crystallizing solvent conditions. The proteins chosen will have a wide variation with respect to molecular weight and crystallizing conditions such as temperature, pH and crystallizing agent type (inorganic salts, PEG's and other organics). The laser scattering solution parameters will be measured in the dilute protein concentration regime, often 10-20 times below protein saturation.

The research approach is to obtain comprehensive measurements of the SLS, DLS and ELS parameters from a set of selected proteins under both crystallizing and precipitating conditions, with particular attention given to the dilute solution regime. The selection of the proteins is significant, and some collaboration with protein crystallographers will be required to totally define the set. Prior verbal agreement for such advisory collaboration has been obtained from Marc Pusey and Dan Carter at the Marshall Space Flight Center in Huntsville, Alabama, Pat Weber at Dupont in Wilmington, Delaware, Alex McPherson at the University of California, Riverside, Franz Rosenberger at the University of Alabama, Huntsville, and Charlie Bugg and Larry DeLucas at the University of Alabama, Birmingham. Use will also be made of the Biological Macromolecule Crystallization Database compiled by Gary Gilliland at the Center for Advanced Research in Biotechnology in Rockville, Maryland. Based on years of experience in performing laser scattering measurements and on the manpower requested in the budget, a target number of twenty proteins is projected for the set, corresponding to roughly one complete set of measurements per protein per month. This amount of time accounts for protein purification procedures as well as repetitions for each of the SLS, DLS, and ELS experiments.

Task Significance:

It is anticipated that a particular solution parameter (or combination of parameters) will be discovered that has quantitative values within a reasonably narrow range for crystallizing conditions and values significantly outside that range for non-crystallizing or precipitating conditions. If such a universal predictor can be proven, then its use will have an immediate impact in the protein crystal growth community in general and microgravity research in particular. The solution conditions for protein crystallization in a microgravity environment should be maximized during ground testing so that a high probability for crystallization is achieved. Having a universal predictor will allow crystallographers to fine tune existing crystallization protocol or discover new conditions to crystallize difficult proteins.

Progress During FY 1996:

A predictor for protein crystallization has been defined in terms of a crystallization slot represented by values of a dilute solution parameter called the osmotic second virial coefficient, B_{22} . The slot includes values of B_{22} between about -2 to -8×10^{-4} mol ml g^{-2} . We have also found that B_{22} is a qualitative predictor for protein solubility for both normal and retrograde solubility behavior. The B_{22} data is being utilized in both passive and active dynamically controlled protein crystal growth experiments.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	2	MS Degrees:	2
PhD Students:	1	PhD Degrees:	0

TASK INITIATION: 7/93 EXPIRATION: 6/97

PROJECT IDENTIFICATION: 962-23-08-21

NASA CONTRACT NO.: NAG8-965

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Ansari, R., Suh, K., Arabshahi, A., Wilson, W., Bray, T., and DeLucas, L. "A Fiber Optic Probe for Monitoring Protein Aggregation, Nucleation and Crystallization." Sixth International Conference on Crystallization of Biological Macromolecules, Hiroshima, Japan, November 1995.

Arabshahi, A., and Wilson, W. "Automated Dynamic Control of Protein Crystal Growth Utilizing Temperature and Laser Light Scattering." 47th Southeast 151st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, Tennessee, November 1995.

Asanov, A., DeLucas, L., Oldham, P., and Wilson, W. "Interfacial Protein Aggregation Related to Crystallization Conditions Studied by Total Internal Reflection Fluorescence." 47th Southeast 151st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, Tennessee, November 1995.

Guo, B., and Wilson, W. "Static and Dynamic Solution Properties of the Protein Ovostatin as Determined by Laser Light Scattering." 47th Southeast 151st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, Tennessee, November 1995.

A Rational Approach for Predicting Protein Crystallization

PRINCIPAL INVESTIGATOR: Dr. W. W. Wilson

Mississippi State University

CO-INVESTIGATORS:

Saebo, S.
Combs, L.Mississippi State University
Kennesaw State College

Task Objective:

The primary objective is to perform light scattering measurements on the proteins BSA and lysozyme to obtain second virial coefficient values in a variety of solvent conditions. The experimental data obtained will then be compared to theoretical results for B_{22} calculated from various solution theories.

Task Description:

Static laser scattering (SLS) will be used to determine the osmotic second virial coefficients, B_{22} , for the proteins in solvents which vary in ionic strength, pH and temperature. McMillan-Mayer solution theory will be used to calculate B_{22} for the same solution conditions.

Task Significance:

The proposed work will determine the feasibility of theoretically predicting the solution conditions that are favorable for protein crystallization. This may eventually allow researchers to develop a theoretical screening method to compliment the various experimental screens.

Progress During FY 1996:

A graduate student has been identified to begin the task, and the materials for Phase I of the work have been obtained. Computer programs have been written for estimating the protein molecule's dipole moment and net charge as a function of solution conditions. B_{22} data for lysozyme as a function of pH and temperature has been determined.

STUDENTS FUNDED UNDER RESEARCH:BS Students: 1
MS Students: 1
PhD Students: 0

TASK INITIATION: 8/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-23-08-34

NASA CONTRACT NO.: NAG8-115

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Hillhouse, T., Arabshahi, A., and Wilson, W. "Using Temperature to Grow Protein Crystals." 16th Annual Undergraduate Chemistry Research Conference, Memphis, Tennessee, March 1996.

Wilson, W. "The Second Virial Coefficient as a Predictor in Protein Crystal Growth." 211th American Chemical Society National Meeting, New Orleans, Louisiana, March 1996.

Wilson, W. "The Second Virial Coefficient as a Predictor in Protein Crystallization." Protein Crystal Growth Conference, Panama City, Florida, April 1996.

Phase Shifting Interferometric Analysis of Protein Crystal Growth Boundaries and Convective Flows

PRINCIPAL INVESTIGATOR: Dr. William K. Witherow

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Sibille, L.

Universities Space Research Association (USRA)

Smith, D.

NASA Marshall Space Flight Center (MSFC)

Task Objective:

The objective of the proposed study is to obtain experimental evidence of several characteristics of a crystallizing protein solution and model their effects on the crystal growth process. The characteristics to be studied include: the presence of concentration gradients during the crystal growth, the extent of the boundary layer from the crystal face, and the effect of buoyancy driven convection on the growth. Phase shifting interferometry (PSI) can provide significant insight to this issue. PSI will produce a visual confirmation of the concentration profile at the boundary layer and concentration values within the depletion region. PSI has the potential to offer a direct visualization of convective flows within proteinic crystallizing solutions.

Task Description:

Mach-Zehnder and Reflection Interferometry with a magnification of up to 1000x will be used to examine growing protein crystals. Phase shifting will be accomplished using an electro-optic phase modulator or a piezo electric mirror. Abel inverse transforms will be used on the resulting phase maps to provide planar phase information.

Task Significance:

Protein crystals are grown to determine the three-dimensional structure of proteins. By utilizing x-ray or neutron diffraction, the collected information allows the direct identification of active sites of the macromolecule, its conformation, and sequence of the amino acids. Sections of very large assemblies of proteins such as structural proteins or viruses can also be crystallized. Crystallization is therefore the starting point of any study aiming at the development of new drugs and the understanding of viral diseases. Crystallization techniques for proteins are now well known, but a biophysical understanding of the growth mechanisms is underdeveloped. This aspect of protein research needs to be expanded as the proteins being studied are more complex and their purification more costly. Since the beginning of the 1980's, tens of proteins have been crystallized in microgravity. Microgravity-grown crystals of several proteins were found to be larger or diffracted with higher resolution than ones previously grown on the ground. These results tend to demonstrate that a reduction of gravity affects the interfacial growth mechanisms which are directly dependent upon the mass transport regime. Convection is known to play a significant role in the growth kinetics of inorganic crystals but its importance is still debated in relation to the crystallization of biological macromolecules. There is little doubt about the existence of convective flows in proteinic solutions, but the flow rates they generate close to the crystal/solution interface and their effect on growth kinetics have not been quantified experimentally. The technique of PSI will allow us to determine these values and provide direct comparison between solutal flows in crystallizing solutions under various levels of gravity. An examination of the flows in the fluid and its correlation with crystal growth will strongly depict the role of microgravity in protein crystal growth.

Progress During FY 1996:

Growing protein crystals have been examined with the use of phase-shifting Michelson-Morley Interferometry. Phase shifting is accomplished using an electro-optic phase modulator. Phase shifting interferometry (PSI) can provide a resolution of at least 1/100 of a wavelength. Phase maps generated by the PSI provide a correlation between crystal growth and convective flow in the growth fluid. Inorganic crystals and protein crystals have been grown. The optical system is a phase shifting Michelson-Morley interferometer being used for this study. The phase shifting algorithm chosen to collect data uses five p/2 phase shifts. By using p/2 phase shifts, the PSI algorithm becomes insensitive to phase shift errors. A computer program has been written that controls the phase shifter, collects the interference data, and calculates the phase map. Initial experiments used sodium chlorate crystals to test the PSI. Strong concentration gradients are formed around sodium chlorate crystals when they grow. The next experiments will grow lysozyme protein crystals. The PSI system is also being developed into a flight system

II. MSAD Program Tasks — Ground-based Research

Discipline: Biotechnology

to be flown on the Mir station next year. After the Mir experiments, ground-based protein crystal growth will be compared with the same type of crystals grown in microgravity. Variations of the PSI system and software developed at MSFC/NASA are being used by groups at the University of California at Riverside and at the De Montfort University in England.

STUDENTS FUNDED UNDER RESEARCH:

BS Degrees: 1
MS Degrees: 0
PhD Degrees: 0

TASK INITIATION: 10/94 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 962-23-08-44

RESPONSIBLE CENTER: MSFC

Characterization of Solvation Potentials Between Small Particles

PRINCIPAL INVESTIGATOR: Dr. Charles F. Zukoski

University of Illinois, Urbana-Champaign

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

A combined experimental and modeling effort is used to characterize how variations in solvent chemical potential alter the states of aggregation of colloidal particles.

Task Description:

The objective of the FY95 program is to develop a combined density fractional theory and Monte Carlo simulation technique to describe the phase behavior of particles where interactions are dominated by solvation forces. In addition, the role of solvent/particle interactions in creating hydrophobic attractions is explored. On the experimental side, direct links are made between interparticle forces and phase behavior through measurements of protein second virial coefficients by light scattering and phase behavior as protein concentration is increased.

Task Significance:

Developing methods which reliably result in high quality protein crystals is of major technological significance in the development of fundamental understanding of biochemical phenomena and the expression of genetically altered therapeutic proteins. In the work carried out here, new methods of controlling protein crystallization are explored. The modeling effort seeks to guide the experimental program by providing understanding of the role of solvation interactions in controlling the state of protein aggregation. The modeling effort has shown that the rarely recognized variable of solvent chemical potential can be used to control protein crystallization behavior. The experimental program is aimed at developing methods of characterizing protein interactions as solvent chemical potential is altered and demonstrating links with crystallization behavior.

Progress During FY 1996:

Our research focusses on understanding the basic physical chemistry of protein crystallization. We follow two approaches. In the first we investigate the fundamentals of protein interactions through studies of the forces between model surfaces using atomic force microscope techniques. In the second approach we investigate how particle interaction potentials control the protein solubility and kinetics of protein crystallization.

Using specially prepared tips, we characterize the hydrophobic interaction between surfaces composed of self assembled monolayers of alkane thiols suspended in a variety of solutions. These studies demonstrate that, for these surfaces, the strength of the hydrophobic interaction increases as the salt concentration increases but decreases in the presence of glycerol. This result suggests that as you increase the strength of the hydrophobic interaction by increasing electrolyte concentration, you expect a lower protein solubility. This is indeed observed and is referred to as "salting out". While this rigin of salting out has been postulated for decades, our studies provide a direct measurement of this effect. On the other hand, as you decrease the strength of the attraction by adding glycerol, the protein solubility should increase. Recently we demonstrated that indeed in the presence of glycerol, protein interactions become less attractive and increasing glycerol concentration increases protein solubility. These results suggest that one must move beyond the classical colloidal interactions of van der Waals and electrostatic forces to describe protein interactions.

In our investigations of protein interactions and solubility we recently demonstrated that protein interactions are well described by an interaction potential which has two adjustable but measurable parameters. This potential is the Adhesive Hard Sphere potential and gives the particles a hard core of diameter d and an attractive well which is very narrow in comparison to d . Due to the short range nature of the attraction, the strength of the attraction can be described in terms of one parameter, T^* , which represents a dimensionless temperature. Large values of T^* indicate hard sphere interactions (i.e., no attractions). As T^* goes to zero, the attractions become very strong. The advantages of the Adhesive Hard Sphere potential are first that the parameters governing the interactions can be determined experimentally and secondly, the phase behavior of Adhesive Hard Sphere systems is well studied from a

theoretical perspective. We determine the particle diameter by dynamic light scattering while T^* can be determined from static light scattering measurements of the particle's second virial coefficient B_2 .

This model suggests particles should display the same solubility if compared at equal values of T^* (or second virial coefficient, B_2). Experiments were carried out where B_2 was varied through changes in supporting solution ionic strength and pH, solution temperature and precipitant (glycerol) concentration. Studies in our laboratory on lysozyme, silicotungstate anions and bovine pancreatic trypsin inhibitor (BPTI) demonstrate that indeed, all these materials have the same solubility at the same value of B_2 . Data gathered from the literature indicate that crystallin (an eye protein) and polymethylmethacrylate particles (one micron in diameter) follow the same behavior indicating the generality of this approach.

When combined, our two pronged attack on understanding protein crystallization opens a window on both the mechanisms of protein interaction and on how to best design solution conditions which give rise to high quality crystals. Our results suggest that by measuring B_2 one can predict protein solubility. By using this nondestructive technique which employs dilute solutions, one is able to tune electrolyte conditions such that attractions are adjusted to a level where high quality crystals can be formed. In addition, our results indicate how proteins interact in solution. The measurements of B_2 suggest that hydrophobic as well as van der Waals and electrostatic forces are important in protein recognition. This observation is not new. However, predicting these interactions remains difficult. Our studies suggest relatively straight forward light scattering measurements can be used to characterize the magnitude of these forces.

While a knowledge of protein solubility is important in growing protein crystals, crystal quality will be controlled by the kinetics of the phase change. In our future studies we will investigate the kinetics of crystal nucleation and growth. Preliminary studies indicate that there is a balance between aggregation producing amorphous clusters and aggregation producing ordered aggregates. Unraveling when each process dominates will be the goal of our next series of investigations.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	1
MS Students:	1	MS Degrees:	3
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 6/93 EXPIRATION: 6/97
 PROJECT IDENTIFICATION: 962-23-08-27
 NASA CONTRACT NO.: NAG8-976
 RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Rosenbaum, D.F. and Zukoski, C.F. Protein interactions and crystallization. *J. Crystal Growth*, vol. 169, 752 (1996).

Rosenbaum, D., Zamora, P.C., and Zukoski, C.F. Phase behavior of small attractive particles. *Phys. Rev. Letters*, vol. 76, no. 150, (1995).

Zukoski, C.F., Rosenbaum, D.F., and Zamora, P.C. Aggregation in precipitation reactions: Stability of primary particles. *Trans. of the Inst. of Chem. Engin., Part A*, vol. 74, 723 (1996).

Effects of Energy Release on Near Field Flow Structure of Gas Jets

PRINCIPAL INVESTIGATOR: Prof. Ajay K. Agrawal

University of Oklahoma

CO-INVESTIGATORS:

Gollahalli, S.R.

University of Oklahoma

Task Objective:

The primary objective of this research is to understand how buoyancy affects the structure of the shear layer, the development of fluid dynamic instabilities, and formation and characteristics of the coherent structures in the near-nozzle regions of burning gas jets. The secondary objective is to understand the role of buoyancy in the flame lifting and reattachment process, evaluate the scaling behavior of diffusion flames, and aid in the development of a theoretical model by providing quantitative temperature data throughout the flame in the absence of buoyancy effects.

Task Description:

The initial phase of this project involves the visualization of near-field flow structures in cold jets and nonsooting flames at the same flow conditions or the same jet exit Reynolds number, allowing the effects of energy release on these structures to be identified by comparison. The experiments will use hydrogen and hydrogen-inert gas mixtures as the fuel with air as the oxidizer. Energy released in the flame will be controlled by varying the hydrogen mole fraction in the jet stream. Attached flames, lifted flames, and flames in the transition region between these two extremes will be studied. Experiments for all cases will be conducted in both normal and reduced gravity.

Task Significance:

The phenomena occurring near the exit of a gas jet nozzle determine burning characteristics and the rate of pollutant generation. The effect of buoyancy on these processes is poorly understood and hence it is difficult to model when designing commercial combustors. This project will study the fluid dynamics of turbulent gas jet combustion, applicable to commercial combustors of this type and may lead to higher efficiencies and lower pollution generation levels.

Progress During FY 1996:

In order to resolve short-duration transient phenomena in the flows under study, a short arc strobing white light source was purchased from Oriel Corporation. This light source was fiber optically interfaced with our color schlieren system. The fiber used was compatible with the single-mode fiber used in the 2.2 second drop tower. Pulsing of this xenon light source was synchronized with the video output using the electronic circuit board built previously. We are now able to obtain 60 fields per second at about 1.2 microsecond pulse duration with sufficient light throughput even at 60% of the maximum capacity. We expect this light source to function well in the more restrictive conditions of the drop tower.

A variety of symmetric exponential filters for the Rainbow Schlieren system were designed and fabricated, along with a calibration procedure wherein the filter is traversed and the motion related to the average hue of the corresponding images. However, this procedure is time consuming and in future, we expect to use a lens combination providing a large focal length to instantly calibrate the filter.

Image processing tools in Fortran to convert schlieren images into reflective index images have been written. These images could also be converted to density, temperature and species concentration images. For fast reacting hydrogen flames, there is a unique relationship between density (or reflective index), temperature and species concentrations based on the chemical equilibrium. Thus, the rainbow schlieren could provide quantitative temperature and species data provided the reactions remain fast. We have pursued this concept using the chemical kinetics code, CHEMKIN. When completed, our imaging processing software integrated with CHEMKIN could provide images of species including H₂, H₂O and O₂, density and temperature. We also plan to experimentally validate this concept using our existing ground facilities together with thermocouples and an oxygen gas analyzer.

The 1G laboratory at the University of Oklahoma came on line after overcoming difficulties such as turbulence in the coflow around the nozzle and ignitor difficulties. Capabilities include ability to vary the fuel flow rate and vacuum level during the test, ability to vary the orientation of the nozzle with respect to the gravity gradient and a schlieren system that remains aligned when that orientation is changed.

The computational effort has focused on validating computed results for simple flow configurations. The validations for steady and unsteady cold jets have been completed. A similar validation effort for chemical kinetic calculations was begun.

A planned research visit during the first two weeks of January was postponed due to the NASA furlough and the destruction of the drag shield. The visit was rescheduled for March, 1996 during the University of Oklahoma's Spring Break. During that visit, Professor Agrawal and a Steven Cherry, Master's student supported under this grant visited LeRC for two weeks of tests. The LeRC-provided ATD schlieren rig performed flawlessly and a total of 17 successful drops were performed. The drop tower staff made the ground floor lab suitably ready for their visit. Working in that area allowed access to a vented gas cabinet which allowed them to study the 1g effects of different flow rates and nozzle diameters prior to dropping. Such extensive work would have been nearly fatally hampered had they been forced to use the system on the 5th level, due to the need to periodically lock out that area during drops. The goal of the drops was to investigate the effects of gravity on hydrogen gas diffusion flames in the laminar, transitional and turbulent regimes. One of the drops included a cold jet and in all of the hot drops but one, the flame was ignited prior to the drop. Light sources were fiber-optically coupled to the rig using an old drop tower communications fiber since it had a larger diameter than the one currently in use. The larger diameter permitted more light to be transmitted.

In the laminar regime, effects of the jet Reynolds number and jet diameter were investigated. The Reynolds number was varied from 100 to 900, in intervals of 200, for a fuel tube of 0.31mm ID (5 drops). The low gravity flames were substantially different from their normal gravity counterparts. Four tube sizes, 0.31, 0.58, 0.84 and 1.19 mm ID were tested at a Reynolds number of 300 (3 drops). The two larger tubes resulted in flame flicker on ground which disappeared in microgravity. The flame flicker was repeatable. Igniting in microgravity (another drop) did not affect this phenomenon. One of these drops was repeated with the strobe light to freeze the flame flicker. Two drops, one with flame and another without the flame, were done with 0.31mm tube at a Reynolds number of approximately 800. In these tests, the flame was laminar while the cold jet became turbulent. In summary, a total of 13 successful drops were completed in this regime alone.

In the transitional regime, the flame became turbulent downstream of a laminar region at the fuel inlet. In hydrogen gas flames, the transition is clearly identified by the flame necking. The transition is very sensitive to the fuel flow rate. Four successful drops in this regime were conducted to identify effects of the tube size, ignition, and light source. In all of these tests, effects of gravity were apparent, at least in the near nozzle region. The data must be examined in greater detail before conclusive statements are made.

Another visit by Prof. Agrawal's students was made to LeRC from June 24 to July 5, 1996. They studied the effect of adding either helium or nitrogen inerts such that a 20 or 40% molar fraction of the inert was obtained. These mixtures were then tested at Reynolds numbers of 700, 1100 and 1500. Following the visit, data reduction was initiated to determine the variation in flame front location and temperature profile between the diluted and non-diluted flames, as well as species concentration and location.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 2

TASK INITIATION: 6/94 EXPIRATION: 5/98
PROJECT IDENTIFICATION: 962-22-05-57
NASA CONTRACT NO.: NAG3-159
RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Al-Ammar, K.N., Agrawal, A.K., and Gollahalli, S.R., "Quantitative measurements in hydrogen flames by rainbow Schlieren imaging." presented at the meeting of the Central States Section of the Combustion Institute, May 5-7, 1996.

Shenoy, A.K., Agrawal, A.K. and Gollahalli, S.R., "Visualizing reacting flow computations by rainbow Schlieren imaging." presented at the meeting of the Central States Section of the Combustion Institute, May 5-7, 1996.

Radiant Extinction of Gaseous Diffusion Flames

PRINCIPAL INVESTIGATOR: Prof. Arvind Atreya

University of Michigan

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of the research is to investigate experimentally and theoretically the radiation-induced extinction of gaseous diffusion flames in microgravity.

Task Description:

Microgravity conditions are required because radiation-induced extinction is generally not possible in normal gravity but is highly likely in microgravity. In normal gravity, the flame generated particulates (eg. soot) and gaseous combustion products that are responsible for flame radiation are swept away from the high temperature reaction zone by the buoyancy-induced flow. Buoyant flow also supports the flame by providing fresh oxygen. In microgravity, however, numerical calculations show that flames are weakened by reduced oxygen supply, accumulation of combustion products and the radiative heat loss from the flame volume associated with emission from the combustion products. This description of microgravity diffusion flames is supported by theoretical models of several types, but has not been adequately demonstrated experimentally.

To investigate radiation-induced extinction experimentally, flames in a spherical geometry are to be used because: 1) the problem is reduced to a one-dimensional case which is much easier to model, 2) the spherical diffusion flame completely encloses the soot formed on the fuel-rich side of the reaction zone, thereby enhancing the radiative loss effect, and 3) for small fuel injection velocities (a practical example being spreading flames over a pyrolyzing solid fuel) microgravity flames tend to adopt a spherical shape. Experiments are to be conducted in the NASA ground-based microgravity facilities using a spherical ceramic burner to reduce conducted heat losses to the burner. The experiments will consist of observations of the transient behavior of these spherical diffusion flames.

The theoretical investigation will continue the development of a model of radiant extinction of diffusion flames that was initiated with previous NASA funding. Realistic theoretical modeling must include not only an adequate estimation of the radiant emissions of the participating gases, but also recognize that the details of the chemical reaction kinetics are possibly quite changed in microgravity from the fast kinetics paradigm successful in modeling normal gravity flames. To develop a useful kinetics scheme, a parallel effort of normal gravity experiments using a low-strain-rate counter-flow diffusion flame will be pursued to obtain the kinetic parameters.

Task Significance:

Diffusion flames are flames in which the fuel and the oxygen are not premixed before reaching the flame, and include useful combustion systems such as home heating, industrial processes and unwanted fires. A great deal of practical information on the design of these practical systems and of the progress of fires has been developed in recent decades, but key participating mechanisms such as gas-phase radiation are not yet understood well enough to be modeled (and engineered) rigorously. This effort will contribute to the understanding of gas phase radiation in gaseous diffusion flames, particularly under conditions where the radiation might cause the flame to be extinguished. This new knowledge is expected to contribute directly to the improved engineering of Earth based and spacecraft fire safety systems.

Progress During FY 1996:

This program task is a new effort in this year, but has a heritage of NASA funding in an earlier NASA Research Announcement award in 1989. During this year results from the earlier work were presented at the 26th International Combustion Symposium. The symposium paper summarizes the results of the normal gravity counter-flow diffusion flame experiments in which the investigators demonstrated an ability to control the location of the soot containing zone from well inside the fuel rich side of the flame to the oxidizer side. The reduced gravity results that were obtained in the previous program were presented at AIAA meetings during that program and are now being prepared for publication in the combustion journals.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 0

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION:

NASA CONTRACT No.: NCC3-482

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Atreya, A., Zhang, C., Kim, H.K., Shamim, T., and Suh, J., "The effect of change in the Flame structure on formation and destruction of soot and NOx in radiating diffusion flames." presented to the 26th International Combustion Symposium, Naples Italy, 1996.

Shamim, T., and Atreya, A., "Dynamic response of radiating flamelets subject to variable reactant concentrations." presented to the Central States Section Meeting of the Combustion Institute, St. Louis, 1996.

Zhang, C., Atreya, A., Kim, H.K., Suh, J., and Shamim, T., "The effect of flame structure on soot inception, growth and oxidation in counterflow diffusion flames." presented to the Central States Section Meeting of the Combustion Institute, St. Louis, 1996.

Zhang, C., Atreya, Shamim, T., A., Kim, H.K., and Suh, J., "Measurements of OH, CH, C2 and PAH in laminar counterflow diffusion flames." presented to the Central States Section Meeting of the Combustion Institute, St. Louis, 1996.

Multicomponent Droplet Combustion in Microgravity: Soot Formation, Emulsions, Metal-Based Additives, and the Effect of Initial Droplet Diameter

PRINCIPAL INVESTIGATOR: Prof. C. T. Avedisian

Cornell University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of the proposed research is to provide insights and data from spherically symmetric combustion, in microgravity, of isolated and unsupported fuel droplets that consist of emulsions and metal-containing additives, and to examine the influence of the initial droplet diameter on the combustion of fuel droplets in microgravity. In addition, the feasibility of using a laser-based light scattering technique for detecting soot formed in spherically symmetric droplet flames in microgravity will be examined. This technique will help assess the effectiveness of additives in influencing soot formation and burning rate processes in droplet combustion.

Task Description:

The burning of multicomponent droplets is complicated by the influence of composition, which can effect the formation of soot, lead to multistage combustion in which one component preferentially vaporizes from the droplet during combustion, or possibly result in the droplet exploding during combustion due to achieving an internal superheat condition. These problems are extremely complicated, especially that of soot formation. The addition of metallic-based additives with hydrocarbon fuels have been shown to suppress soot formation. A CCD camera coupled with an image intensifier for the purpose of recording UV light emissions from a burning droplet will be measuring the droplet flame diameter and a laser light scattering technique will be set-up to provide a quantitative measure of soot formation. The experiments will be conducted in a drop tower at Cornell that provides approximately one second of reduced gravity.

Task Significance:

Little data have been provided regarding the spherically symmetric burning of unsupported droplets of multicomponent fuels or emulsions. Depending on the relative concentrations and volatilities of the components, and their miscibility, multi component fuels exhibit peculiar, unsteady-burning characteristics. The importance of examining these burning characteristics is that most practical fuels which are burned in combustion-powered devices or incinerators are multicomponent in nature, usually miscible, but sometimes immiscible (emulsions).

If the mechanism for an influence of initial droplet diameter on spherically symmetric droplet burning can be understood and predicted for the "simple" spherically symmetric droplet flame, this information may be useful for providing insights into the influence of initial droplet size on soot formation in a convective environment. Metal additives can create the potential for significant reductions in particulate emissions by the possible effect of the ions produced on the nucleation and agglomeration of soot particles, and their possible oxidation; their effect in the droplet flames, especially in the spherically symmetric configuration, is unknown.

Progress During FY 1996:

Continuing work centers around three activities: 1) analysis of emulsion droplet experiments, 2) development of full chemistry for heptane droplet experiments, and 3) design of a droplet levitation scheme. On the first, a paper is to present the results of experiments done on free emulsion droplet combustion. The current plan is to include a comparison of the preferential vaporization process observed for emulsions with one observed in prior publications for miscible mixtures. On the second, publication was accepted by Combustion Science and Technology of the effect of water addition on heptane droplet combustion which included complex chemistry modeling. On the third, a droplet levitation technique for the Cornell 1 second drop tower is currently being optimized as compared to a previous droplet deployment scheme of shooting a droplet into a projectile and then as it reaches the apex of its trajectory the droplet experiment would be dropped down the tower. This scheme has demonstrated itself to be unreliable for emulsion fuel droplets.

II. MSAD Program Tasks — Ground-based Research

Discipline: Combustion Science

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 1

TASK INITIATION: 8/95 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-22-05-49

NASA CONTRACT NO.: NAG3-179

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Jaeleson, G.S. and Avedisian, C.T., Modeling of spherically symmetric droplet flames including complex chemistry: Effect of water addition on n-heptane droplet combustion. Combustion Science and Technology, vol. 115, pp. 125-149 (1996).

Gas-Phase Combustion Synthesis of Metal and Ceramic Nano-Particles

PRINCIPAL INVESTIGATOR: Prof. Richard L. Axelbaum

Washington University, St. Louis

CO-INVESTIGATORS:

Chao, B.-H.

University of Hawaii

Task Objective:

To gain a greater understanding of particle synthesis in flames, with emphasis on understanding and advancing the technology of sodium/halide combustion for synthesis of metal and ceramic nanopowders.

Task Description:

The combustion of halides in atmospheres of sodium vapor will be studied by employing the spherically symmetric geometry afforded by microgravity combustion. Specifically we will (1) simulate and study droplet burning (employing a porous sphere) for single- and two-component halides in a sodium or sodium/ammonia atmosphere, (2) synthesize nano-particles of a variety of metals and ceramics, and (3) study particle formation, growth and multi-component coating processes. Experiments will also be performed in normal gravity, to the extent that they allow the microgravity experiments to be efficiently performed and to understand the effects of gravity on the flame and particle formation. Modeling will accompany the porous sphere experiments, and predicted and measured flame stand-off distances, temperature profiles and particle size distributions will be compared.

Particles in the flames will be thermophoretically sampled by rapidly inserting TEM grids into the flame zone. These particles will then be analyzed by TEM for size and elemental composition. The sampling experiments will be performed so that complete profiles of particle size and composition are obtained as a function of radial distance from the porous sphere.

The detailed modeling of particle formation, growth and coating in spherically symmetric nonpremixed systems is a unique contribution of this research. With the one-dimensional, spherically symmetric flame, the plan is to incorporate diffusion flame structure as well as detailed particle dynamics. These results will be compared to the experimentally obtained profiles of particle size. Particle dynamics will be evaluated by Monte Carlo simulations and solving the general dynamic equation (GDE) by the sectional method which performs a population balance to evaluate particle history.

Task Significance:

Flame synthesis processes are presently responsible for production of over 2.5 million tons of powders annually in the U.S. Recent studies have shown that novel flame processes can be employed to synthesize powders for a new class of materials - nanostructured materials. When powders produced in these flames are consolidated, the resulting nanostructured materials can have highly desirable mechanical, electronic and magnetic properties, finding applications in defense, electronics, medicine, and aerospace. This program is an investigation of the sodium/halide flame process for producing metal and non-oxide ceramic nanoparticles. A controlled study of these flames in the nonbuoyant environment provided by microgravity, will result in a greater understanding of the process, and an ability to optimize its use.

Progress During FY 1996:

The grant was officially awarded on June 25th, 1996. So far, the PI and one of his Ph.D. students, Lee J. Rosen, have been working on designing the sodium/halide droplet burner experiment. They are following the design of the established drop-tower rigs for droplet burning, with modifications for the unique requirements of sodium/halide flames. Ordering of materials and equipment has begun.

Washington University allocated an additional 700 sq. ft. of laboratory space to the PI for this project and the laboratory has been renovated in preparation for development and testing of the droplet burner experiments.

The Co-I and PI have begun modeling the flame and particle dynamics. The graduate student that has been involved in this project, Jose I Huertas, is expected to complete the Ph.D. program in January, 1997. A first-year Ph.D.

student, Zhen Sun, will take over the modeling effort in September. Presently, the Monte Carlo method is being employed to model particle dynamics, and a program has been completed and tested for modeling single component aerosols. A two-component, multi-dimensional model is under development.

The Co-I and PI completed a draft of an analytical study of soot particle inception in flames. The study employs a high-activation-energy asymptotic analysis with three-step kinetics. The results demonstrate the critical role that flame structure can have on particle formation in flames, and how, by varying structure, particle inception can be accelerated or suppressed.

The PI visited the Co-I in June, 1996. Discussions included 1) defining immediate and long term objectives, 2) allocating responsibilities, and 3) extensive technical discussions.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-22-00

NASA CONTRACT NO.: NAG3-191

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Axelbaum, R.L., Lottes, C.R., Huertas, J.I. and Hariprasad, S., "Gas-phase combustion synthesis of aluminum nitride powders." Proceedings of the 26th Symposium (International) on Combustion, Naples, Italy, July 1996.

Presentations

Axelbaum, R.L., Huertas, J.I., Lottes, C.R., Hariprasad, S., Sastry, S.M.L., "Nanophase W and W-Ti composite via gas-phase combustion synthesis." 1996 ASME Mechanics and Materials Conference, Johns Hopkins University, Baltimore, June 12-14, 1996.

Axelbaum, R.L., Lottes, C.R., Huertas, J.I. and Hariprasad, S., "Gas-phase combustion synthesis of aluminum nitride powders." presented at the 26th Symposium (International) on Combustion, Naples, Italy, July 1996.

Axelbaum, R.L., Lottes, C.R., Huertas, J.I., Rosen, L.J. and Hariprasad, S., "Synthesis of aluminum nitride nano-particulates via gas-phase combustion." Third International Conference on Nanostructured Materials, Kona, Hawaii, July 8-12, 1996.

Axelbaum, R.L., Lottes, C.R., Huertas, L.J. and Hariprasad, S., "Gas-phase combustion synthesis of nano-particulates of W and W-Ti composite." Third International Conference on Nanostructured Materials, Kona, Hawaii, July 8-12, 1996.

Development of Advanced Diagnostics for Characterization of Burning Droplets in Microgravity

PRINCIPAL INVESTIGATOR: Dr. William D. Bachalo

Aerometrics, Inc.

CO-INVESTIGATORS:

Sankar, S.V.

Aerometrics, Inc.

Task Objective:

This research is intended to develop rainbow thermometry for quantitative radial temperature measurements in burning droplets and use Morphologically-Dependent Resonances for quantification of the radial regression rate. Both of these techniques will be developed using devices amenable for use in one of NASA's reduced gravity aircraft; this hardware will be delivered to LeRC at the end of the project.

Task Description:

Rainbow thermometry utilizes the angular dependence of rainbow location. In other words, given a known droplet composition, the location of the rainbow generated by that drop when illuminated with a monochromatic source will give the refractive index of the drop, and thus, its temperature. Instrumentation and software will be developed that will permit quantitative droplet temperature measurement.

Morphologically-Dependent Resonances occurs when the droplet diameter is an integral number of wavelengths of the illumination source. As the droplet size regresses due to combustion, this condition will be repeatedly met, causing the droplet to periodically "shine." The rate at which this occurs will give the diameter regression rate and will be accomplished using the same hardware as for the rainbow thermometry.

Task Significance:

Droplet combustion is an economically vital phenomenon occurring in liquid-fueled engine combustion, which includes both mobile and stationary combustors. Optimization of such designs has been hindered due to insufficient knowledge about the nature of combusting droplets. This project will develop analytic instrumentation that will allow measurement of the radial temperature distribution and size of combusting droplets. While the tools to be developed can be used in either normal or reduced gravity, the latter admits the use of much larger droplets and dramatically increases the information yield of the experiment.

Progress During FY 1996:

After several discussions with Dr. DeVon Griffin of NASA LeRC, the following has been agreed to in terms of the deliverable for the contract. It was agreed that the possibility of using the high power diode laser available at NASA Lewis might not be very practical for this program. Instead we have decided to use a 30 mW polarized diode laser (instead of the He-Ne). The increased power (compared to the He-Ne) and the greater sensitivity of the CCD at the diode laser wavelength will be beneficial. It is also possible to increase the amount of light incident on the CCD sensor by using a shorter CCD array (1024 instead of 2048). The physical size of the CCD array will be 2048 but the camera will be jumpered to read only the first 1024 pixels. Therefore, if it is desired to use 2048 at a later time, it will be possible to re-jumper the camera. We will have to study how this setup performs during a flight test. We believe we will be able to measure the droplet size and temperature. If, and how well, we are able to measure the regression rate with this setup is to be seen. At a later time we can replace the 30 mW diode laser with the NASA Lewis diode laser or some other laser and see whether it does improve the situation.

In the original statement of work, Aerometrics agreed to loan NASA Lewis the necessary frame-grabber for flight testing. The XPG-1000 Power Grabber from Dipix is currently being evaluated for the current application. The Dipix board features four analog input channels, but also allows the expansion to acquire images from digital cameras. Camera acquisition modules connect various types of cameras to the frame-grabber board. Several cameras can be interfaced at once. Standard data rates are up to 20 MHz, with optional modules available for higher data rates. The main reason the Dipix board is attractive for the present application is that it offers a unique combination of cache memory to optimize data acquisition and processing. The unique architecture of the board allows for concurrent acquisition and processing, maximum advantage of the parallel processing architecture of the TMS

320C40 DSP processor. The board also features an optional per-processing module for arithmetic image operations prior to its handling by the DSP.

The frame-grabber was successfully interfaced to a Loral-Fairchild CAM1800. Since this camera was not directly supported by Dipix, extensive software and hardware testing had to be undertaken to successfully integrate the camera and the board. We are currently try to save the CCD line scan output and at the same time perform a real-time brightest pixel detection operation. If we succeed in this, then the peak detection based rainbow signal processor can be replaced by the Dipix frame grabber. This will allow us to perform real-time peak detection and at the same time save the digitized rainbow signals for post-processing. This requires more software development and hardware testing and we are receiving extensive technical support from Dipix in this regard. Since we don't have the frame grabber operating in this mode yet, our short term goal is to use the Dipix frame grabber in conjunction with the peak detection based rainbow signal processor for droplet temperature measurement. The Dipix frame grabber and the peak detection based rainbow signal processor will be controlled by two separate PCs. The data acquired by the two computers (one measuring the peak rainbow location and the other digitizing the complete rainbow signal) will be properly synchronized by means of an 4-bit event counter that is output by the Dipix board and that is interfaced to the peak detection based rainbow signal processor.

The data acquired by the two computers will be post-processed using the LabView environment. A virtual signal processor is being developed in LabView to process the data acquired by the two computers. The digitized rainbow images will be saved as a TIFF file on one computer and the size, velocity, rainbow peak location, and count number will be saved in the second computer as an ASCII file. The LabView virtual signal processor will read the two files and process the data using different signal processing criteria including FFT, peak detection, thresholding, etc. The LabView environment will be used to identify suitable validation criteria for the measurement at hand. The development of the LabView virtual signal processor is currently under development.

In June, 1996, Aerometrics determined that the hardware was essentially complete and invited the COTR, Dr. DeVon Griffin of LeRC, to visit the Aerometrics facility for a demonstration of the capabilities. As demonstrated, the hardware measured the diameter of a burning droplet, the diameter regression rate and the bulk refractive index of the droplet. Dr. Griffin made two suggestions for hardware modification to increase the ease of use. The hardware was delivered to LeRC during the last part of October.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 8/94 EXPIRATION: 12/96

PROJECT IDENTIFICATION: 962-22-05-43

NASA CONTRACT NO.: NAS3-272

RESPONSIBLE CENTER: LeRC

Ignition and Combustion of Bulk Metals in Microgravity (Ground-Based Experiment)

PRINCIPAL INVESTIGATOR: Prof. Melvyn C. Branch

University of Colorado, Boulder

CO-INVESTIGATORS:

Daily, J.W.

Fiechtner, G.J.

University of Colorado, Boulder

University of Colorado, Boulder

Task Objective:

The project is an analytical and experimental investigation of the mechanisms of ignition and combustion of metal pellets under low-pressure oxygen atmospheres in a low-gravity environment. Innovative features of the research, which is an outgrowth of a preceding normal-gravity and elevated-gravity study, are a non-disturbing radiative-ignition source and advanced diagnostics for determination of surface and gas temperatures, flame characteristics, and metal-oxide surface morphology.

Task Description:

The experimental study uses an apparatus and techniques developed by the Principal Investigator and research associates to investigate the entire process of metal combustion, starting from heat-up and ignition to post-combustion quenching. The metal fuels are in the form of bulk pellets rather than the typical non-representative powder forms. Two unique features of the apparatus are the 1000-W, short-arc-lamp ignition source, which eliminates the contamination of the reaction zone and ignites all metal specimens in a clean and reproducible manner, and the compact combustion chamber with full optical access for non-disturbing measurements. The observation of the metal surface during ignition and combustion is achieved through high-speed photography. Metal-oxide combustion specimens are recovered after each test and analyzed physically and chemically by electron microscopy and spectroscopic methods.

Metal combustion is strongly affected by gravity level, particularly in microgravity, because the changed mobility of the liquid phase in a varying convective environment affects the surface exposure of the burning metal. Testing at varied gravity levels also simulates the environment of oxygen handling systems in launch, orbit, and reentry conditions of spacecraft engines and vehicles. The experimental test matrix includes normal-gravity reference tests and elevated-gravity tests in a centrifuge apparatus, all conducted at the facilities of the University of Colorado. The principal experiments are the low-gravity tests, conducted in the NASA Lewis Research Center Reduced Gravity Airplane Facility (DC-9).

Concurrent analyses involve modeling of the metal heating, ignition, and combustion processes as influenced by gravity level and oxygen pressure. The initial findings were verified by the experimental normal-gravity measurements of metal temperature rise, with excellent agreement. The experimental results also contribute information necessary to add surface and gas-phase reaction rates and conductive, convective, and radiative heat transfer into the modeling.

Task Significance:

The study is the first approach to the investigation of ignition and combustion of bulk pure metals under conditions that facilitate the interpretation of the temperature and compositional histories. The practical application of the results promise improvement in the handling and fire safety of oxidizer pumping and storage systems for spacecraft and industrial applications.

Progress During FY 1996:

The experiments in the current year concentrated on the ignition, combustion, and post-combustion behavior of two metals in pure oxygen at a total pressure of 101 kPa (1 atm). Titanium (Ti) and magnesium (Mg) were chosen to illustrate heterogeneous, or surface oxidation and homogeneous, or gas-phase oxidation characteristics, respectively. The two metals also provide a contrast in differing melting and boiling temperatures, heats of combustion, oxide formation processes, and flame temperatures.

Tests were conducted in two separate campaigns on the NASA Lewis Research Center Reduced Gravity Airplane Facility (DC-9). The tests consisted basically of heating a 4-mm diameter by 4-mm high metal pellet in a combustion vessel with a radiant lamp. The first sequence of tests, which had diagnostics measuring chamber pressure, pellet temperature, and high-speed motion picture flame visualization, was conducted in the previous year. The second sequence, conducted in the current year, added spectroscopic surveys and covered additional test variations.

Magnesium showed a more rapid heat-up in low gravity compared to normal gravity. The metal expands upon heating in low gravity, promoting evaporation and oxidation. The metal collapses upon heating in normal gravity, due to gravitational settling.

Titanium showed a slower rate of heat-up and ignition in low gravity compared to normal gravity. The lack of convective flow away from the solid may reduce the absorption of oxygen in low gravity.

Temperature histories enabled the definitions of critical temperatures, the point where surface oxidation equals heat losses from the sample, and ignition temperatures. The high applied heating rates and large internal conduction losses in the experiments, both in normal and reduced gravity, generated critical and ignition temperatures that were several hundred degrees above the values obtained in previous isothermal experiments. Because of high conduction losses, however, the ignition temperatures varied little in low gravity from those in normal gravity, despite the reduced convection. The accumulation of condensed oxide particles in the low-gravity flame front produced a previously unreported unsteady explosion phenomenon in bulk magnesium flames. These spherically symmetric explosions seem to be driven by increased radiation heat transfer from the flame front to an evaporating metal core covered by a porous, flexible oxide coating.

Propagation rates of the molten interface on titanium and of ignition waves on magnesium in reduced gravity are in close agreement with theoretical predictions based on a diffusion/convection-controlled reaction. The experimental results have revealed the significant role of gravity on the burning of metals, and they are now being used as the database for future experiments to be conducted with different metals at various pressures, oxygen concentrations, and gravity levels.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 2
MS Students: 0
PhD Students: 1

TASK INITIATION: 12/94 EXPIRATION: 11/97

PROJECT IDENTIFICATION: 962-22-05-30

NASA CONTRACT NO.: NAG3-168

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Abbud-Madrid, A., Branch, M.C., and Daily, J.W., Ignition and combustion of bulk metals at normal, elevated, and reduced gravity. Univ. of Colorado Report CCR No. 95-05 - Annual Technical Report, (CASI N96-17775), NASA CR-200007, (December 10, 1995).

Abbud-Madrid, A., Branch, M.C., and Daily, J.W., On the burning behavior of radiatively ignited titanium at low gravity. AIAA Paper 96-0262, (Jan 15-18, 1996).

NASA Tech Briefs

Branch, M.C., Daily, J.W., and Abbud-Madrid, A., Ignition and combustion of bulk metals in a microgravity environment. NASA Tech Brief, CCR No. 96-09, (September 16, 1996).

Presentations

Abbud-Madrid, A., Branch, M.C., and Daily, J.W., "Ignition and combustion of bulk titanium and magnesium at normal and reduced gravity." 26th International Symposium on Combustion, The Combustion Inst., Naples, Italy, Paper 443, July 29-Aug. 2, 1996.

Modeling of Microgravity Combustion Experiments - Phase II

PRINCIPAL INVESTIGATOR: Prof. John D. Buckmaster

University of Illinois, Urbana-Champaign

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective is modeling of existing microgravity experiments for improving our understanding of the fundamental physics. Specific areas of interest include smoldering combustion, premixed flammability studies, radiation effects, and diffusion flame instabilities.

Task Description:

Microgravity combustion experiments amenable to modeling are identified, and analytical and numerical models are developed from first principles for various systems and configurations. Model predictions are compared with experimental results and necessary adjustments and enhancements are incorporated into the models. Precise quantitative comparisons are made using numerical simulations where possible.

Task Significance:

Modeling provides invaluable physical insights into the experimentally observed behavior. This study is done in close collaboration with experimentalists with the goal of providing a clear understanding of the underlying physics.

Progress During FY 1996:

The paper entitled "Role of Slip in the Generation of Acoustic Instabilities in Gas Turbines," by M. DiCicco and J. Buckmaster, (completed in December 1993 and submitted to the Journal of Propulsion and Power with a slightly different title), was published in Jan. 1996. The Abstract of the paper reads: "Slip affects the response time of fuel sprays to acoustic fluctuations in a gaseous flow field. This paper describes how gaseous fuel is released by evaporation as an oscillating response to the acoustic velocity fluctuations, and so contributes to acoustic instability. The paper discusses the differences due to the evaporation characteristics of various fuels (JP-4, JP-5, and D-2) as well as the effect of droplet size, inlet air temperature, air speed, and Reynolds number on mass response. For example, it is shown that instability will be driven harder at lower frequencies, higher gas velocities, and increased liquid volatility."

The paper entitled "Quenching of Reverse Smoulder," by D. Lozinski and J. Buckmaster was published in Combustion and Flame in late 1995. The Abstract of the paper reads: "A simple model of reverse smoulder in a porous medium is analyzed using asymptotic methods. When the only chemical reaction is exothermic oxidation, the burning rate is a single-valued function of the blowing rate, increasing from zero to a maximum, and then returning to zero. When endothermic pyrolysis is added to the description, the burning rate is double-valued for blowing rates less than some maximum. Beyond this maximum there are no solutions. The upper branch of the double-valued solution is the physically relevant one. On it, for certain choices of parameters, the burning rate increases from zero to a maximum, and then decreases until quenching occurs at the maximum blowing rate. This behavior mimics experimental observations by Torero, Fernandez-Pello, and Kitano (1993)."

The paper entitled "Extinction and other Topics in Smoldering Combustion," by J. Buckmaster and D. Lozinski was published in the Proceedings of the Third Asian-Pacific International Symposium on Combustion and Energy Utilization in late 1995. The Abstract of the paper reads: "An elementary model of premixed smoldering has been analyzed which predicts a monotonic rise in the burning rate as the blowing rate is increased, followed by a monotonic fall to zero. When endothermic pyrolysis is included in the model the response displays a turning point beyond the maximum, corresponding to quenching at a non-zero burning rate. This response is in concordance with experiment. A stability analysis characterized by a fast-time scale defined by the thin reaction zone shows that heat losses towards the burnt material generated by pyrolysis tend to destabilize, whereas an effective Lewis Number less than 1, defined by the gas-phase Lewis Number and the densities of the two phases, tends to stabilize. For modest blowing rates stability is assured, but a portion of the response prior to the static quenching point can be unstable."

The paper entitled "An elementary discussion of forward smouldering," by J. Buckmaster, and D. Lozinski was published by Combustion and Flame in early 96. The Abstract of the paper reads: "We describe an elementary model of one-dimensional unsteady forward smouldering, purged of all unnecessary physics. Following work of Dosanjh and Pagni, a late time solution is constructed, characterized by two reaction fronts - an exothermic oxidation front, an unusual kind of diffusion flame; and an endothermic pyrolysis front. It is shown that the flame temperature and the ratio of the speeds of the two fronts relative to the solid are independent of the blowing rate, in agreement with data obtained by Ohlemiller and Lucca. The structure of the oxidation front is described in the context of 1-step Arrhenius kinetics, and it is shown that leakage of solid reactant through the front is possible, but not leakage of oxygen. An elementary pyrolysis structure is also examined which reduces to the frontal model in a certain limit, and clarifies its nature."

A paper entitled "A Theory of Shallow Smoulder Waves," by J. Buckmaster was published by the IMA J. of Applied Mathematics in early 96. The Abstract of the paper reads: "A smoulder wave traveling through a porous solid slab is analyzed as a small Stefan number free-boundary problem, assuming that the wave depth is small compared to its length. It is shown that the wave aspect ratio $AR (= \text{length/depth})$ depends on two parameters: the Peclet number UL/D where ρ is the air density, U the wave-speed, L its length, and D is the diffusion coefficient of oxygen; and the stoichiometric volume ratio of solid/air, which is small on account of the large solid/air density ratio. Assuming Peclet numbers near 1, it is shown that when free-stream convection is modest the aspect ratio will be large. When convection is large, however, no general statement is possible, although shallow waves can occur for realistic parameter values. Wave shapes are calculated, as are the oxygen and temperature fields. For large convection velocities the results are in qualitative agreement with numerical simulations, and with experimental observations."

A paper entitled "Radiation Losses in Hydrogen-Air Flame-Balls," by J. D. Buckmaster was published in the Proceedings of the Central States Section of The Combustion Institute under the Proceedings Title of "Combustion Fundamentals and Applications." The meeting was held in St. Louis, Missouri in May 5-7, 1996. This Proceedings does not have an ISBN number.

A paper entitled "Edge-Flames and Their Stability," by J. Buckmaster was published by Combustion Science and Technology in 96. The Abstract of the paper reads: "Flame sheets that arise in non-premixed combustion often have edges. The leading edge of a flame spreading over a fuel-bed, solid or liquid, is one example. The edge of a hemi-spherical candle flame in microgravity is another. We construct a one-dimensional model which contains some of the essential physics of these edge-flames, and use this model to describe stationary solutions and their stability. The model corresponds to a new class of combustion waves which resemble deflagrations in some respects yet exhibit important differences. Thus, in a uniform flow, wave-like solutions are possible with positive, negative or vanishing wave-speeds, depending on an assignable Damkohler number. At large activation energy, reaction is concentrated primarily in a thin region (the edge) but it persists, in diminished form, behind the edge. This residual reaction plays a key role in defining the flame- or edge-temperature which, in turn, controls the dynamics of the structure. The familiar Lewis-number stability boundaries of deflagrations are present in modified form and provide tentative explanations of pulsations and cellular structures that have been observed experimentally."

An extended abstract entitled "Modeling Microgravity Combustion Phenomena," by J. Buckmaster was published in late 95 in the Proceedings of the Eastern States Meeting of the Combustion Institute, the matching text to Buckmaster's plenary talk. The role of analytical modeling in combustion is illuminated by a discussion of flame-balls, smoldering combustion, and edge flames. This Proceedings does not have an ISBN number.

A manuscript entitled "Edge-flame-holding," by J. Buckmaster and R. Weber was accepted for presentation at the 26th Int. Combustion Symposium, and will be published in the Proceedings. The Abstract of the paper reads: "Non-premixed flame sheets often have edges, in which case we call such structures edge-flames. They have wave like properties in the sense that stationary structures can exist which travel at a well-defined speed relative to the flow on the reaction free side of the edge. Edge speeds can be positive or negative. Recently a one-dimensional model of edge-flames has been proposed by Buckmaster, and here we apply this model to an edge-flame that is fixed in the teeth of an accelerating flow by diffusive interaction with a burner rim. Blow-off occurs if an assigned Damkohler number is too small, and for values of this number greater than some minimum there are two solutions. A stability analysis shows, as expected, that the solution branch for which the stand-off distance increases with

Damkohler number is unstable. These results are familiar, but have not previously been deduced in the context of a simple model with exact, albeit asymptotic, solutions."

A manuscript entitled "Edge-Flames," by J. Buckmaster was submitted to the Journal of Engineering Mathematics for a special combustion issue being organized by Norbert Peters. The Abstract of the paper reads: "Edge-flames arise in non-premixed combustion, and include the familiar triple, or tribrachial flames. They can exist for all Damkohler numbers for which the upper branch of the S-shaped response of the underlying diffusion flame exists, and have negative propagation speeds (corresponding to failure waves) when the Damkohler number is close to the quenching value, positive speeds (corresponding to ignition waves) when the Damkohler number is large. A previously described one-dimensional model of edge-flames is here applied to a number of new situations. These include: a description of unbounded edge-flames, for unit Lewis numbers, over the entire range of Damkohler numbers; a description of unbounded edge-flames when one of the Lewis numbers differs from unity, for a restricted range of Damkohler numbers, for which it is shown that propagating edge-flames of stationary structure may not exist; and an analysis of an edge-flame near a wall, sans flow between the wall and the flame."

Prof. Buckmaster has been appointed to the editorial board of a new journal to be published by the Institute of Physics called "Combustion Theory and Modeling."

Prof. Buckmaster was asked to organize and chair a session on 'Combustion Problems' for the 19th International Congress of Theoretical and Applied Mechanics, to be held in Kyoto, Japan, August 25-31, 1996. He will present a talk in this session entitled 'Applications of a one-dimensional model of edge-flames'.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	1
PhD Students:	1	PhD Degrees:	0

TASK INITIATION: 3/95 EXPIRATION: 3/98

PROJECT IDENTIFICATION: 962-22-05-31

NASA CONTRACT NO.: NAG3-170

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Buckmaster, J., A theory of shallow smolder waves. IMA J. of Applied Mathematics, vol. 56, pp. 87-102 (1996).

Buckmaster, J., Edge-flames and their stability. Comb. Sci. & Technol., vol. 115, pp. 43 (1996).

Buckmaster, J., and Lozinski, D., An elementary discussion of forward smoldering. Combustion and Flame, vol. 104, pp. 300-310 (1996).

DiCicco, M., and Buckmaster, J., Role of slip in the generation of acoustic instabilities in gas turbines. J. of Propulsion and Power, vol. 12, no. 1, pp. 34-40 (1996).

Lozinski, D., and Buckmaster, J., Quenching of reverse smolder. Combustion and Flame, vol 102, pp.87-100 (October 1995).

Proceedings

Buckmaster, J., "Modeling microgravity combustion phenomena." Invited Plenary Lecture, The Eastern States Meeting of the Combustion Institute, October 16-18, 1995.

Buckmaster, J., "Smoldering combustion." AIAA 96-0258, AIAA 34th Aerospace Sciences Meeting & Exhibit, Reno, NV, 1996.

Buckmaster, J., "Edge-flame-holding." Proceedings of the 26th Symposium (International) on Combustion, Naples, Italy, July 1996.

Buckmaster, J., and Lozinski, D., "Extinction and other topics in smoldering combustion." Proceedings of the Third Asian-Pacific Int. Symp. on Combustion and Energy Utilization, Vol. II, Combustion Fundamentals, pp. 426-431, Hong Kong, December 1995.

Buckmaster, J. D., "Radiation losses in hydrogen-air flame-balls, combustion fundamentals and applications." Proceedings of the Central States Section of The Combustion Institute, pp. 316-321, 1996, St. Louis, Missouri, May 5-7, 1996.

Presentations

Buckmaster, J., "Modeling microgravity combustion phenomena." Invited Plenary Lecture, The Eastern States Meeting of the Combustion Institute, October 16-18, 1995.

Buckmaster, J., "Smouldering combustion." AIAA 96-0258, AIAA 34th Aerospace Sciences Meeting & Exhibit. Reno, NV, 1996.

Buckmaster, J., "Applications of a one-dimensional model of edge-flames." Combustion Problems session, the 19th International Congress of Theoretical and Applied Mechanics, Kyoto, Japan, August 25-31, 1996.

Buckmaster, J. and Weber, R., "Edge-flame-holding." presented at the 26th Symposium (International) on Combustion, Naples, Italy, July 1996.

Buckmaster, J. D., "Radiation losses in hydrogen-air flame-balls." Combustion Fundamentals and Applications, Proc. of the Central States Section of The Combustion Institute, pp. 316-321, 1996, St. Louis, Missouri, May 5-7, 1996.

A Numerical Model for Combustion of Bubbling Thermoplastic Materials in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Kathryn M. Butler

National Institute of Standards and Technology

CO-INVESTIGATORS:

Yang, J.C.

National Institute of Standards and Technology

Kashiwagi, T.

National Institute of Standards and Technology

Task Objective:

The objective of the proposed work is to improve our fundamental understanding of the combustion characteristics of thermoplastic materials in microgravity.

Task Description:

To improve our fundamental understanding of the behavior of burning thermoplastic materials in microgravity, a time-dependent, three-dimensional numerical model will be developed to predict the temperature field, burning rate, and bubble bursting characteristics of these materials.

The proposed numerical model includes the dynamics of bubble growth and migration, heat transfer through the condensed material, the chemistry of gasification, and coupling to the gas phase. This model is an extension of a model currently being developed at NIST to study the swelling and heat transfer properties of intumescent heat-resistant materials. The thermoplastic material is initialized as a volume of highly viscous material in which a number (on the order of 1000 to 10000) of bubble nucleation sites are randomly distributed. A heat flux is applied to the outer surface and the energy equation is solved to determine the temperature field. When the temperature at a given bubble site exceeds the degradation temperature of the polymer, the bubble begins to grow at a rate determined by the relevant chemistry and physics. The migration of each bubble due to the effect of the local temperature gradient on viscosity and surface tension, to the flow fields of surrounding bubbles, and to buoyancy (when gravity is a factor) is computed, and the loss of mass due to expulsion of fuel vapor and liquid droplets at the outer surface is modelled. A separate model will study details of the bursting process. Gas phase mechanisms will be calculated in sufficient detail to adequately represent the coupling between the flame and the surface of the burning thermoplastic sample.

The proposed model will be used to study the results of a separate, current NASA project on the combustion of a PMMA sphere in microgravity. Temperatures from the model will be compared with measurements from thermocouples embedded in the sphere, and the nucleation and migration of bubbles and the size of the sphere as a function of time will be compared with enhanced images from high-resolution cameras. In ground-based trials of the experimental apparatus the PMMA sample remains sufficiently transparent during combustion to observe bubble nucleation and motion. The experiment will be helpful in verifying the model, and experience with the model may suggest new directions for solid combustion experiments in microgravity.

Task Significance:

Recent microgravity experiments on combustion of thermoplastics, including velcro made of nylon and electrical wire insulation, have pointed out a fire hazard unique to low gravity. Chemical reactions within the bulk of certain burning thermoplastic materials generate internal bubbles, which grow and migrate until they burst at the surface and eject fuel and fuel vapor into the surroundings. Under normal gravity conditions, the primary danger of fire spread by contact with burning thermoplastics is from the dripping of the molten material. In microgravity, however, the forceable ejection of molten fuel droplets and fuel vapor uniquely enhances fire growth by transporting burning material in random directions, threatening the safety of the crew and spacecraft. The results of this study will improve our fundamental understanding of the combustion characteristics of thermoplastic materials in microgravity.

Progress During FY 1996:

The interagency agreement to support this work was funded in June of 1996.

Improvements have been made in hydrodynamics and heat transfer submodels describing the behavior in the immediate vicinity of the bubble. Transient effects have been added to the calculation of heat transfer for a bubble of low thermal conductivity expanding in a viscous liquid. The results indicate that the current quasi-steady representation of the bubble as a simple dipole in the temperature field is reasonable at the high thermal gradients of interest.

The temperature field surrounding the bubble has been linked to the hydrodynamics calculations. The forces that cause the bubble to migrate toward higher temperature regions now take into account the distortion caused by the low thermal conductivity of the bubble.

Dr. Butler attended the Third Microgravity Fluid Physics Conference in Cleveland on June 13-15 to make contacts with researchers and to give a lunchtime talk at NASA Lewis on this project.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 1/00

PROJECT IDENTIFICATION:

NASA CONTRACT No.: C-320033-

RESPONSIBLE CENTER: LeRC

Heterogeneous Combustion of Porous Solid Fuel Particles Under Microgravity: A Comprehensive Theoretical and Experimental Study

PRINCIPAL INVESTIGATOR: Prof. H. K. Chelliah

University of Virginia

CO-INVESTIGATORS:

Miller, F.

Case Western Reserve University

Task Objective:

There are two objectives to this research. First, experiments will be conducted to determine the oxidation rates, flame stand-off distances, and surface temperatures of a variety of porous, carbonaceous particles as they burn in microgravity (some normal gravity tests will also be performed). In addition, measurements of the pore distribution of char particles will be carried out. Secondly, the experimental data will be used to help validate a detailed numerical model which will be further developed for this work to provide a basis for separating the effects of physical parameters from finite-rate kinetics.

Task Description:

Carbon particles in the size range 200 to 1500 μm of various porosities will be ignited and burned in a small combustion chamber which will serve to control the ambient conditions. We plan to employ laser heating of the particles, which will be fiber supported, to achieve rapid ignition. During the combustion process, the particles will be viewed with two video or high-speed movie cameras to determine their regression rate and to measure the flame location relative to the particle surface. In addition, a two-color pyrometer will measure the particle surface temperature. Some particles will not be completely combusted, but will be quenched and saved to perform measurements of the pore structure using gas-adsorption and mercury porosimetry and will be studied under an electron microscope to determine pore changes. The microgravity experiments will be conducted in the two NASA Lewis Drop Towers, as well as on the DC-9 aircraft for longer burning particles. The numerical model currently in existence will be further developed for the spherically symmetric case of porous particles. The model will include finite-rate homogeneous and heterogeneous kinetics, two-phase equations to account for combustion in the internal pore structure, and thermal radiation. For small particles, the current code will also be extended to include transient effects. Once completed, the model will be validated by checking it against the experimental data compiled as described above.

Task Significance:

Coal combustion currently supplies about one half of the electricity generated in this country, and the use of coal is expected to increase in the coming decades. Much of the coal burned is in the form of small, porous particles, the combustion of which occurs in two stages: rapid pyrolysis followed by slow char oxidation. The details of the latter are still not completely understood, nor have there been detailed comparisons to a complete numerical model. These experiments and model, which will benefit from the spherical symmetry that microgravity will allow, will significantly extend our level of knowledge of this process. Furthermore, the oxidation of some metal particles is also a similar phenomena which the model can later be applied to.

Progress During FY 1996:

We have begun background reading of some previous experiments to help us choose components for our drop rig. A camera and magnifying lens have been bought and tested. Carbon particles (200 μm ϕ) have been obtained and have been successfully drilled to accommodate a ceramic (10 μm ϕ) tether, which has also been received. Work has begun on a tensioning system. The numerical model has begun to be modified to account for the pore structure.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/96 EXPIRATION: 7/00

PROJECT IDENTIFICATION: 962-22-00

NASA CONTRACT NO.: NAG3-192

RESPONSIBLE CENTER: LeRC

Buoyancy Effects on the Structure and Stability of Burke-Schumann Diffusion Flames

PRINCIPAL INVESTIGATOR: Prof. L.- D. Chen

University of Iowa

CO-INVESTIGATORS:

Stocker, D.P.

NASA Lewis Research Center (LeRC)

Task Objective:

The general goals of the proposed research are to improve our understanding of (1) the influence of buoyancy on co-flow diffusion flames, e.g., Burke-Schumann diffusion flames, and (2) the effects of buoyancy on vortex-flame interactions in co-flow diffusion flames. The overall objectives of the proposed work are to:

1. Verify the zero-gravity Burke-Schumann model and the gravity-dependent Hegde-Bahadori extension.
2. Investigate the flame stability in a buoyancy-dependent flow-field as affected by the co-flow oxidizer.
3. Examine the state relationships of co-flow diffusion flames.
4. Study flow vortex and diffusion flame interactions.

Task Description:

D. Stocker (NASA LeRC) has the lead responsibility for the microgravity testing which is being conducted in ground-based facilities and in a Glovebox investigation, ELF - Enclosed Laminar Flames, that is scheduled for the USMP-4 mission. The Glovebox investigation will be focused on a study of the influence of buoyancy on the flame's stability (i.e., lift-off and blow-off) limits. The ground-based testing is being conducted in the 2.2 Second Drop Tower, and the DC-9 aircraft. Future tests may also be conducted in the Zero-Gravity Facility, most likely using the rig developed for the Gas-Jet Diffusion Flames (GDF) experiment, since only limited modifications would be required.

Task Significance:

The 1928 Burke-Schumann diffusion flame analysis is of fundamental and historical interest, and can be found in many, if not all, introductory combustion textbooks in the U.S. Experimental validation of this zero-gravity model will be an important contribution to combustion science, and it is likely to be referenced in future textbooks. Additionally, the study results could lead in the long-term to improved engine or furnace efficiency and reduced pollutant emissions.

Progress During FY 1996:

A. Numerical Modeling

The time-accurate numerical model that was developed during the last report period (FY 1994-95) is used for prediction of such quantities as the flame structure, the NO_x and soot formation, and radiative transport in axisymmetric jet diffusion flames. The numerical model adopts a semi-implicit time marching and a finite-difference method for spatial discretization. A higher-order accurate and oscillation free solution is obtained by applying a higher-order differencing scheme and flux-corrected transport to the convection flux. Validation on the current model is performed by computing the Smith and Hutton problem and the Burke-Schumann diffusion flames. Theoretical assessment on the order of accuracy of temporal and spatial differencing for multi-dimensional flame modeling is given by Sheu and Chen (1996). The results suggest that a higher-order accurate and oscillation free scheme is required for spatial order of accuracy; whereas a first-order time differencing scheme is adequate for temporal accuracy for the time-dependent laminar Burke-Schumann diffusion flames.

A finite-rate chemistry model for methane oxidation has been implemented in the numerical model for prediction of flame structure and NO_x emission from the flame. A single-step global and a four-step reduced mechanisms are considered. Evaluation of the four-step reduced mechanism is carried out by comparing the predictions with experimental data and computational results in the literature. Satisfactory agreement is obtained even though a coarse grid distribution is used.

The reduced mechanism is used to study the flame stabilization, the state relationship of species concentrations and temperature, and the effects of molecular transport in a Burke-Schumann diffusion flame. The simulation proposes that the spike in local integrated heat release can be used as a criterion for flame stabilization. The heat release

criterion is consistent with the onset of CH radicals in the flame reported in the literature. The simulation predicted nearly universal state relationships for concentrations of major species of CH₄ in the fuel-rich region, O₂ in the fuel-lean region, CO₂, H₂O and temperature, but not for H, H₂ or CO. The predicted state relationships remain unchanged with or without the presence of buoyant acceleration in the flame. The effects of molecular transport are also studied. The results show that the preferential diffusion in enthalpy flux and the differential diffusion of species decrease the temperature at locations near the flame tip. When both effects are considered in the simulation, the predicted maximum flame temperature shifts from the flame-tip location to the flame shoulder region.

An extended reduced mechanism based on a four-step reduced reaction for methane oxidation and a thirty-step reaction for NO_x formation is developed. Using the current model coupled with the extended reduced mechanism, the state relationships of nitrogen species concentrations, the buoyancy effects on NO_x emission, and the relative importance of thermal NO and NO₂ formation mechanisms to the total NO_x emission are investigated. No universal state relationships are obtained for the nitrogen species examined, suggesting that chemical reactions involving these nitrogen species keep varying along the axial distance. The presence of the buoyant force results in an increase of the mass flow rate of NO in the post-flame region and a decrease of the NO₂ mass flow rate. The molar flow rates of NO and NO₂ (i.e., the NO_x emission) remain constant for both normal-gravity and zero-gravity predictions. The simulation also shows that the thermal NO only accounts for 13% of the total NO_x prediction. The prompt NO, NO₂ and N₂O formation are therefore important in the methane-fueled Burke-Schumann diffusion flame studied.

The proposed reduced mechanism for nitrogen chemistry is tested. The simulation shows that NO, HCN, and NO₂ should be modeled as reactive species for prediction of NO_x formation in a methane-fueled laminar diffusion flame. Validation of the current numerical model coupled with the reduced mechanism for nitrogen chemistry is performed by comparing the simulation with that using the thirty-step NO_x formation mechanism. Nearly identical results are obtained between the results predicted by both mechanisms.

The effects of radiant energy transport with presence of soot particles in a methane-air diffusion flame are studied. The radiative transfer is accounted for by implementing the Discrete-Ordinates method in the calculation. The soot volume fraction is predicted by a calibrated soot oxidation model. The simulation on the relative importance of soot oxidant species suggests that OH and H₂O are the dominant oxidant species in the fuel-rich and flame-tip regions, and O₂ is the dominant species in the fuel-lean region. This conclusion agrees with the experimental data in the literature, except for H₂O that is not considered in their soot oxidation model.

The effects of wall emissivity are examined using three wall emissivity values, 0.2, 0.85, and 1.0. The results show that the predictions of the flame temperature and soot volume fraction are not affected by the three wall emissivity values studied. The calculation of the interactions between soot particles and radiant energy transport shows that soot particles are the major contributor to the radiative transport in the methane-air diffusion flame studied. The presence of soot particles is found to increase radiative heat loss and decrease the temperature prediction. The effects of radiant energy transport on the flame structure are also examined. The calculation shows that the state relationships of species concentrations are not altered by the radiative transport and the presence of soot particles in the flame. The state relationships of temperature, however, are altered at axial locations where soot particles are predicted. Therefore, the approximations of universal state relationships are not appropriate for flames with radiant energy transport and presence of soot particles.

The major conclusions of the present study are summarized as follows:

1. A higher-order accurate and oscillation free scheme is required for spatial order of accuracy; whereas a first-order time differencing scheme is adequate for temporary accuracy for prediction of near-laminar Burke-Schumann diffusion flames.
2. The four-step reduced mechanism for methane oxidation, and the extended reduced mechanism for methane oxidation and NO_x formation are demonstrated to be promising alternatives to detailed chemistry models for prediction of the diffusion flame studied.
3. The evaluation of the proposed reduced mechanism for nitrogen chemistry shows that NO, HCN, and NO₂ should be modeled as reactive species for prediction of NO_x formation in a methane-fueled laminar diffusion flame.
4. The thermal NO only accounts for 13% of the total NO_x prediction. Therefore, the prompt NO, NO₂ and N₂O formation are important to the Burke-Schumann diffusion flame studied.

5. Nearly universal state relationships are obtained for concentrations of major species of CH₄ in the fuel-rich region, O₂ in the fuel-lean region, CO₂, H₂O and temperature, but not for H, H₂, CO and the nitrogen species examined.
6. For the methane-fueled diffusion flame studied, in addition to OH and O₂, H₂O is also a dominant soot oxidant species.
7. The approximations of universal state relationships are not appropriate with the presence of radiative heat transfer and soot particles in the diffusion flame studied.

B. Experimental

A proposal for a Glovebox investigation of the stability of Enclosed Laminar Flames (ELF) was approved in early 1996 for full development towards flight on the USMP-4 mission in October 1997. Fabrication and assembly of the prototype hardware was completed at this time. The ELF hardware consists of a module, and two parts boxes, containing the control box, electrical cables, spare ignitors, and fuel bottles. Nitrogen-diluted methane will be burned in a co-flow of air, produced by an electric fan. The hardware is instrumented with two fixed thermocouples at the nozzle, and a harp-like rake of five thermocouples and 26 SiC fibers. The rake can be rotated to various radial positions by the astronaut. There are three parameters that can be varied: (1) fuel flow via a mass flow controller, (2) air velocity, and (3) temperature rake position. These will be displayed and recorded on video, along with three thermocouple readings. The other thermocouple readings will be recorded onto the audio track of the glovebox video. Preliminary studies of the ELF Glovebox investigation were conducted in microgravity in June 1996 using the prototype hardware on the DC-9. These results showed that the visual flame and the thermal field become wider in reduced gravity, as was anticipated. Normal-gravity tests were conducted to quantify the temperature of the hand guard located at the ELF exhaust, and the mean and rms velocities of air flow inside the ELF duct. Testing is being conducted of the ELF flame in a reduced-pressure environment of 0.7031 bar (or 10.2 psia), and will be followed by the condition of 0.3 bar. Numerical simulation is in progress for the ELF flame in 0g at a fuel-jet velocity of 0.8 m/s and a co-flowing air velocities of 0.2, 0.4, 0.6, and 0.8 m/s. The results will be used to identify conditions for temperature profile measurements during the Glovebox investigation on the USMP-4 mission.

Experiments have been conducted in normal gravity to study the structure of methane-fueled Burke-Schumann diffusion flame (BSDF) in reduced pressure using a scanning thermocouple probe. The measurements show that the local maximum temperatures at axial locations increase with decreasing pressure, and with apparent decreases of the soot formation. The decrease of soot concentration is evident from the decrease of soot agglomeration on the thermocouple probe and the loss of luminosity at reduced pressures. Decrease of soot volume fraction is believed to be responsible for the higher local stoichiometric temperature resulting from a lower radiative heat loss (relative to the heat release) in reduced-pressure environments. The measurements also show the flame tip temperature is lower than the maximum temperature in the shoulder region, a combined effect of non-unity Lewis number and radiative heat loss.

The lift-off conditions of the methane-fueled laminar BSDF in a reduced pressure environment are characterized. A cylindrical BSDF burner was placed inside a vacuum chamber, with an vertically upward fuel jet surrounded by a coflowing air. The coflowing air was set to have the same velocity as the fuel jet at the burner inlet. The data were taken at reduced pressures while keeping the (fuel and air) mass flow rate unchanged. The flame was seen to lift from the burner when the system pressure was reduced. The stabilization height increased with decreasing system pressure. A laminar and stable flame was observed for the conditions tested until the blow out limit was reached. The luminous flame shape becomes cusp-like near the blowout limit, showing a premixed flame like behavior. The concept of local extinction of a lifted flame in still air (Peters and Williams, 1983) was extended to the coflowing air environment, and with the extinction scalar dissipation rate modified to account for the reduced pressure effects. The extended scalar dissipation-rate concept was successfully used to correlate the current data of the laminar BSDF in reduced pressures, along with the experimental data of turbulent jet diffusion flames in a still environment. The correlation coefficient of Peters and Williams was adopted in current analysis. Similar to the 1983 paper, the current data showed size dependence of the results; the size dependence of current measurements was observed for stabilization heights located within the six fuel-jet diameters from the fuel-tube exit.

A new burner assembly was designed at NASA Lewis for use in upcoming drop tests in the 2.2-Second Drop Tower. The new burner will have a 10x10 cm chimney with rounded corners, circular nozzles of up to 12 mm in

diameter, a retractable ignitor, and 5-cm wide schlieren-quality windows. The burner will also allow for use of (1) a slot nozzle up to 75 mm in length, (2) a nozzle mounted for cross-flow studies, or (3) multiple nozzles to study flame interaction. A hot-filament will be incorporated into the fuel nozzle to track flow oscillations in pulsed flame tests. Temperature rake(s) with thermocouples and SiC fibers will be designed for use within the chimney, and provisions have been made for mounting other instrumentation in and out of the duct.

Normal-gravity testing on the stabilization of laminar jet diffusion flames in cross flow was conducted. A transverse fuel jet was positioned on a horizontal plane and issued into a vertically up-ward flowing air flow. Temperature measurements and flame visualization were made of a methane-fueled diffusion flame. The visualization showed that for a fixed fuel-jet velocity, transition from an attached to a detached flame occurred when the cross-flow air velocity was increased. The detached flame usually stabilized in the wake-region of the fuel tube and anchored at the tube; the flame tip became nearly non-luminous. A higher cross-flow velocity was required when the fuel-jet velocity is increased. Substantially lower temperatures were measured at locations near the lower flame boundary compared to the measurements near the upper flame boundary for both the attached and detached flames. The temperature data suggested flame stretch at the lower luminous flame boundary and flame compression at the upper flame boundary. The temperature data also suggests loss of characteristics of the diffusion flame when detachment occurs.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	1
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 6/94 **EXPIRATION:** 6/98

PROJECT IDENTIFICATION: 962-22-05-63

NASA CONTRACT NO.: NAG3-159

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:
Thesis

Bang, H.-N., An experimental investigation of jet diffusion flames: flame response and stabilization in cross-flow, M.S. Thesis. The University of Iowa, Iowa City, Iowa, (July, 1996).

Dissertation

Sheu, J.-C., Numerical Simulation of Burke-Schumann Diffusion Flames Using Finite-Rate Chemical Kinetics, Ph.D. Dissertation. The University of Iowa, Iowa City, Iowa, (May, 1996.).

Journals

Sheu, J.-C. and Chen, L.-D., A higher-order accurate model for the simulation of time-dependent variable density flow. AIAA J., vol. 34, no. 10, (1996).

Proceedings

Bang, H.-N. and Chen, L.-D., "An experimental investigation of laminar jet diffusion flame stabilization in cross-flow." Proceedings of the 1996 Spring Technical Meeting of the Central States Section of The Combustion Institute, St. Louis, MO, pp. 175-280, May 5-7, 1996.

Sheu, J.-C and Chen, L.-D., "A reduced mechanism for prediction of NO_x emission from atmospheric methane-air diffusion flame." Proceedings of the 1996 Spring Technical Meeting of the Central States Section of The Combustion Institute, St. Louis, MO, pp. 52-57, May 5-7, 1996.

Presentations

Lee, Y.G. and Chen, L.-D., "Effects of Damkohler number on the lifted methane laminar diffusion flames at reduced pressure." presented at the KSEA 6th Midwest Regional Conference, Iowa City, Iowa, June 21-22, 1996.

Sheu, J.-C and Chen, L.-D., "A numerical investigation of the effects of radiative heat transfer on the structure of a gaseous diffusion flame." Paper No. 96-3091, the 1996 AIAA/ASME/ASCE/SAE Joint Propulsion Conference, Lake Buena Vista, FL, 1-3 July, 1996.

Gravitational Effects on Premixed Turbulent Flames: Microgravity Flame Structures

PRINCIPAL INVESTIGATOR: Dr. Robert K. Cheng

Lawrence Berkeley Laboratory

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The overall objective of this experiment is to investigate the influence of gravity on premixed turbulent flame propagation.

Task Description:

The emphasis of this experimental program will be on measuring flame wrinkle scales and imaging mean flowfield properties of conical Bunsen-type flames and rod-stabilized V-flames. Laser diagnostics will be used to obtain statistical scalar and velocity information to evaluate parameters suitable for predicting the effects of gravity on turbulent premixed flames. DC-9 parabolic flights will be performed as well as parallel laboratory experiments. The research effort is an extension of a previous NRA effort entitled "Gravitational Effects on Premixed Turbulent Flames."

Task Significance:

This research effort will provide insight to determine significant processes through which gravity affects flame properties such as flame speed and flame structures. The results will be used to determine the gravity-influenced limit for premixed turbulent flames. Such knowledge is valuable for guiding the development of turbulent combustion models to include the effects of gravity. This study will contribute to resolving the inconsistencies that exist between experiments and theories. If better understood, turbulent combustion can be exploited to enhance burning rates and volumetric power density in many heating and power generating systems.

Progress During FY 1996:

Two journal papers are being prepared for submission to Combustion and Flame. The first paper focuses on the effects of bouyancy on the overall features of laminar and turbulent v-flames. The analysis of the flame angles from the schlieren images show the effects of bouyancy disappears at Reynold's number around 2000. The results indicate a diminishing effect in the near field. The effects of bouyancy to the far field region is shown qualitatively by the Schlieren but can not be quantified due to the limitation of the technique. The PI also compared the bouyancy induced v-flame pulsation frequency to those observed in conical flames. While the conical flame pulsation frequencies correlates with Re #, those of v-flames do not. This is due to the differences in flame geometry and in particular, a significant change in the size of the products plume.

This analysis is important to understanding how bouyancy is coupled to the flowfield. The PI's earlier discovery of a unique laminar flame that is stabilized by bouyancy has helped to identify the relevant parameters to describe the balance between bouyancy forces and momentum. The purpose of the present analysis is to apply the knowledge for comparing the +g and -g v-flame flowfields. For -g v-flames it was demonstrated quantitatively that the flow acceleration in the products can be attributed to bouyancy. This is a new insight as previous works have assigned the acceleration to be flow convergence. Using this approach, the flow deceleration in the -g can also be associated with bouyancy forces. Here, it was possible to quantify the bouyancy effect. The main reason being that the +g flames are plan-symmetric. Therefore, 2D momentum equations apply. In -g, significant divergence requires 3D treatment. The PI's 2D estimations are inadequate. As a consequence of this analysis, the PI is exploring the use of simple phenomenological models to describe the flowfield that will lead to better insight into microgravity flames.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 3/96 EXPIRATION: 3/98

PROJECT IDENTIFICATION: 962-22-05-32

NASA CONTRACT NO.: C-3200012

RESPONSIBLE CENTER: LeRC

Combustion of Interacting Droplet Arrays in a Microgravity Environment

PRINCIPAL INVESTIGATOR: Dr. Daniel L. Dietrich

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

Kitano, K.

Hokkaido National Industrial Research Institute

Task Objective:

This research program involves the study of one-dimensional and two-dimensional arrays of droplets in a buoyant-free environment. The purpose of the work is to extend the data base and theories that exist for single droplets into the regime wherein droplet interactions are important.

Task Description:

The emphasis of the present investigation is experimental, although comparison will be made to existing theoretical and numerical treatments when appropriate. Both normal-gravity and low-gravity testing will be employed, and the results compared.

The normal-gravity testing will utilize the classical suspended droplet technique; single droplets and droplet arrays will be supported on 125 μm optical fibers in a combustion chamber where the ambient environment can be controlled. The low-gravity testing will employ droplets suspended on 15 μm Si-C fibers again in a combustion chamber where the ambient environment can be changed.

Task Significance:

The results of this work will improve models on spray combustion, wherein droplets seldom burn individually (the combustion history of a droplet is strongly influenced by the presence of the neighboring droplets).

Progress During FY 1996:

The Fiber Supported Droplet Combustion glovebox experiment (FSDC) was performed in October 1995. Individual droplets with diameters ranging from about 2-5 mm were burned under microgravity conditions in air at 1 bar with an ambient temperature of 300 K. Each droplet was tethered by a silicon carbide fiber of 80 or 150 μm to keep it in view of video recording, and, in some tests a forced air flow was applied in a direction parallel to the fiber axis. Methanol, two methanol-water mixtures, two methanol-dodecanol mixtures and two heptane-hexadecane mixtures were the fuels. Droplet and flame diameters were measured as functions of time. The prediction that methanol droplets extinguish at diameters that increase with increasing initial droplet diameter is verified by these experiments. In addition, the quasi-steady burning rate constant of the heptane-hexadecane mixtures appears to decrease with increasing droplet diameter; obscuration consistent with very heavy sooting, but without the formation of soot shells, is observed for the largest of the droplets. Forced convective flow around methanol droplets was found to increase the burning rate and to produce a ratio of downstream to upstream flame radius that remained constant as the droplet size decreased, a trend in agreement with earlier results obtained at higher convective velocities for smaller droplets having larger flame standoff ratios. The data are being compared to theoretical and numerical models of droplet combustion and will lead to improved modelling of single droplet combustion phenomena.

In addition to the FSDC work, experiments on simulated single droplet combustion were conducted aboard the DC-9 aircraft using the porous sphere technique. Tests were also conducted at the Japan Microgravity Center for single droplets and droplet arrays. The work shows, consistent with the FSDC results, that radiative loss is important for large single droplet combustion. Decane flames which at smaller sizes (~ 1 mm) are sooty and luminous become dim blue with diminished soot production at larger droplet sizes. Evidence of radiative extinction was also observed in the aircraft tests, although g-jitter makes the results hard to interpret. Finally, the effects of g-jitter on the sphericity of the flame were explained by a new sphericity parameter which compares the buoyant velocity to the Stefan (blowing) velocity at the flame front.

Experiments on droplet arrays in Japan show that for a three droplet array, the burning rate of the center droplet is smaller than that of the end droplets. The burning rate of the center droplet increases as the inter-droplet spacing

increases. This is true for heptane, methanol and decane, although the magnitude of the change is different for each fuel.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1.5
MS Students: 0
PhD Students: 0

TASK INITIATION: 10/94 EXPIRATION: 12/98

PROJECT IDENTIFICATION: 962-22-05-33

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Haggard, J.B., Dryer, F.L., Nayagam, V., Shaw, B.D., and Williams, F.A., Droplet combustion experiments in spacelab. The Combustion Institute, (1996).

Struk, P. and T'ien, J.S., Large droplet combustion and extinction experiment conducted in reduced gravity aboard an aircraft. Microgravity Science and Technology, (1996).

Presentations

Haggard, J.B., Dryer, F.L., Nayagam, V., Shaw, B.D., and Williams, F.A., "Droplet combustion experiments in spacelab." Twenty-Sixth Symposium (International) on Combustion, Naples, Italy, 1996.

Internal and Surface Phenomena in Heterogeneous Metal Combustion

PRINCIPAL INVESTIGATOR: Dr. Edward L. Dreizin

AeroChem Research Laboratories, Inc.

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The project is an experimental and analytical study of the combustion of isolated, freely falling droplets of aluminum, titanium, and zirconium — metals chosen to represent a range of burning behavior. The study emphasizes the processes of oxygen penetration within the burning droplet and its influence on combustion rate, temperature history, and product composition.

Task Description:

The study uses a novel apparatus, developed by the Principal Investigator, that generates and ignites metal droplets through electrical-arc discharges with consumable, pure-metal electrodes. This insures repeatable formation and ignition of uniform metal droplets with a controllable initial temperature and velocity. The burning droplets are subsequently quenched to terminate the reaction at prescribed stages of the combustion. Test variations include those of temperature, droplet size, and atmospheric oxygen concentration for three selected metals, aluminum (Al), titanium (Ti), and zirconium (Zr), chosen to illustrate a range of surface and vapor-phase combustion characteristics. The experimental data cover droplet observations, droplet temperatures and diameters as functions of time, and chemical and metallurgical analyses of the internal composition of the quenched, solidified specimens.

In microgravity, the absence of settling forces permits the precise control of the droplet motion, which greatly aids in the interpretation of the droplet-diameter and droplet-temperature histories. In this respect, the quantitative results of the first phase of the testing in normal gravity serve as guidelines for subsequent low-gravity experiments. The low-gravity phase of the study is being conducted in the NASA Lewis Research Center Reduced-Gravity Airplane Facility (DC-9), using the novel ground apparatus with structural modifications to meet the specialized requirements for airplane installation.

Concurrent with the experimental studies, analytical studies verified by the experimental results will model the processes occurring in metal-droplet combustion to provide a theoretical foundation of surface and internal transport, reaction-rate phenomena, and product distribution for the selected metal fuels.

Task Significance:

The generation of monodisperse metal droplets allows the conduct of microgravity metal-combustion experiments that are analogous to those of microgravity liquid fuel-droplet combustion. In contrast to the essentially homogenous liquid-fuel droplet, however, the internal structure of the metal droplet can be altered by controlled quenching and rapid freezing. This characteristic can greatly influence temperature histories and energy release. The results of the study thus have practical application to the safety and improved performance of metallized fuels, which are widely used as solid rocket propellants in, for example, the Shuttle Solid Rocket Boosters and the Titan IVB Strap-ons.

Progress During FY 1996:

In the current year, the testing of Ti and Zr combustion in the normal-gravity phase concluded. The facility modification, safety assessment, and test matrix development for low-gravity testing were also completed.

Experiments conducted during the first year of effort confirmed the nature of the two stages of metal-droplet combustion. The first stage is that of the formation of a liquid metal-oxygen (air) solution within the burning droplet. The second stage is that of the reaction to form the stoichiometric metal oxide. Earlier work on boron-wire combustion interpreted through this mechanism was reported during the current year.

The compositional histories of Ti particles obtained through controlled quenching at various times within the combustion process show distinct Ti-O and Ti-N burning systems. This metal burns heterogeneously, that is, in

the condensed solid and liquid phases within the particle. Compositional histories confirm the stated two-stage nature of combustion as a function of time, where oxygen dissolves in the pure Ti and Ti suboxygen matrices with increasing concentration until the mechanism changes to the formation of stoichiometric TiO₂. These same results and interpretations apply to Zr combustion histories. Both metals also exhibit uptakes of nitrogen during combustion. For Zr, the composition-temperature histories are adequately interpreted through reference Zr-O phase diagrams, where the oxygen concentration is that of "equivalent oxygen", i.e., O plus N. This analysis fails to interpret the phase behavior of Ti combustion in air, however.

Improved reproducibility of results was an important achievement of the test program. Various changes in the electronic triggering for droplet generation and ignition contributed to reduce the testing problems. A high-speed video camera was added to the diagnostic array. A goal that was attained is the generation of droplets with initial velocities less than 25 cm/s, sufficiently slow to enable the imaging of essentially quiescent combustion.

The testing at low gravity will begin in October 1996 in the NASA Lewis Research Center DC-9 Airplane Facility. The apparatus was modified to provide a compact installation, with substantial improvements for rigidity and strength. The modified apparatus was tested for vibrational response on a shake stand at the AeroChem facilities. Test sequences, safety analyses, and accommodations were submitted to the NASA Lewis Research Center for the low-gravity airplane tests. All have been approved by NASA.

The low-gravity testing will be confined to a single metal, aluminum, for validation of the concurrent modeling. The droplet-generator mechanism translates by spring action as the arc is struck to impart a motion to the droplet that is counter to the path of fall. In normal gravity, the droplet has some residual motion, but in low gravity, the droplets are near-motionless. Thus the droplet remains within the field of view of the spectrometer and imaging camera for at least several seconds during the combustion process to aid the observation of the droplet, flame, and smoke shell. Moreover, the minimization of convection flows in low gravity influences the composition and homogeneity of the reacting and quenched droplet.

The modeling studies in progress concentrate on aluminum. Aluminum combustion takes place in the vapor phase, and thus the combustion mechanism must include evaporation as well as oxygen transport and combustion. The analyses for aluminum are nearly complete, and model results are being compared to experimental data.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/94 EXPIRATION: 1/98

PROJECT IDENTIFICATION: 962-22-05-46

NASA CONTRACT NO.: NAS-3-27

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Dreizen, E.L., Experimental study of stages in aluminum particle combustion in air. Comb. and Flame, vol. 105, pp. 541-556 (June 1996).

Presentations

Dreizen, E.L. and Calcote, H.F., "A new mechanism of boron ignition: Through the formation of a saturated B-O solution." Paper presented at the Fall Tech. Meeting of the Eastern States Sec., The Combustion Inst., Worcester MA, October, 1995.

Molodetsky, E.E., and Dreizen, E.L., "High-temperature oxygen dissolution in liquid zirconium." Presented at the Materials Research Society 1995 Fall Meeting, Boston MA, November 27 to December 1, 1995.

Molodetsky, I.E. and Dreizen, E.L., "High temperature oxygen dissolution in liquid zirconium." Paper presented at the Fall Meeting, Materials Research Society, Boston MA, November 27, - December 1, 1995.

Molodetsky, I.E.; Dreizen, E.L.; and Law, C.K. "On the evolution of particle temperature and internal composition for zirconium burning in air." Paper 442, presented at the 26th Symposium (International) on Combustion, The Combustion Inst., Naples Italy, July 29 - August 2, 1996.

Interaction of Burning Metal Particles

PRINCIPAL INVESTIGATOR: Dr. Edward L. Dreizin

AeroChem Research Laboratories, Inc.

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This project is an analytical and experiment study of the combustion of metal-particle clouds, in terms of individual-particle motions, interactions, and combustion, aerosol combustion, and overall energy transport and radiation. Experiments in microgravity are highly advantageous since the absence of settling motions permits the generation, containment, and observation of stable metal aerosols composed of relatively large particles, of the order of 50 to 300 μm in dimension.

Task Description:

The experiments involve the fluidization of relatively large, uniform spherical metal particles, of the order of 100 μm in dimension, under microgravity and igniting the resulting aerosol using a high-energy chemical igniter or a laser beam. Metal fuels will include vapor-burning magnesium and aluminum and surface-burning titanium and zirconium. Experimental parameters to be controlled are particle concentration, oxygen partial pressure, and diluent-gas composition.

The flame propagation and details of individual particle combustion and interparticle interactions will be studied using high-speed cinematography with microscope enlargements. If the aerosol is formed in a relatively thin sheet, 5 to 20 mm in thickness, the individual particles should then be visible. Thus, the images will show the motions of burning particles, the individual flames, smoke clouds, and particle interactions. Other diagnostics planned are ionization probes to detect electrical charges induced during combustion, chamber pressure, and oxygen consumption to determine completeness of combustion. In addition, combustion products will be collected and analyzed for microstructure and composition.

Experimental results will be assessed to determine individual-particle and aerosol temperature histories and burning rates. It is expected that a model can be derived for generalized prediction of transport and reactions in cloud and spray combustion.

Task Significance:

The behavior of burning metal-particle clouds, distinct from that of conventional liquid sprays, has never been studied experimentally before. The microgravity environment, which stabilizes the metal-particle aerosols, provides the opportunity for the novel testing regime. The study offers considerable benefits. Results can provide information necessary for the improvement of the performance of metallized solid propellants in space propulsion systems and for far-ranging terrestrial applications, such as in pyrotechnics and thermite welding.

Progress During FY 1996:

The project initiated in the final months of the fiscal year. The chamber for the aerosol containment was designed and constructed. The activating loud-speaker system, ignition source, and some of the diagnostics are now in place. The chamber has a "floor" made of 1/32-inch silicone rubber sheeting for efficiency in transmitting vibrations. Glass beads, 150 to 260 μm in size, were used for calibration of the range of frequency and acoustic power necessary to fill the chamber volume adequately.

Preliminary testing initiated with the dispersion and ignition of magnesium powders at loads of 2 to 5.5 g in a 0.625-L volume. Electrically heated tungsten wires appeared to provide the most dependable means of aerosol ignition.

II. MSAD Program Tasks — Ground-based Research

Discipline: Combustion Science

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-22-05-71

NASA CONTRACT No.: NAS3-960

RESPONSIBLE CENTER: LeRC

Flame-Vortex Interactions Imaged in Microgravity

PRINCIPAL INVESTIGATOR: Prof. James F. Driscoll

University of Michigan

CO-INVESTIGATORS:

Dahm, W.J.A.

Sichel, M.

University of Michigan

University of Michigan

Task Objective:

The objective of this research is to investigate a method that will provide high quality, quantitative, color enhanced digital images of a vortex exerting aerodynamic strain on a flame under microgravity conditions. This will be used to:

1. Quantify how the vortex distorts the flame;
2. Define the degree of flame curvature;
3. Show how preferential diffusion affects temperature profiles.

Task Description:

The fundamental interaction between turbulence and chemistry in a combustion process will be studied by interacting a repeatable, well-defined vortex, or variable size and strength vortex, with premixed and nonpremixed flames. The complicating effects of buoyancy will be eliminated by employing the NASA LeRC 2.2 Second Drop Tower. High quality, quantitative, color enhanced 2-D images will be obtained of the temperature field, the flame emission, and the mixture fraction (nonpremixed case). Results will be compared to full Navier-Stokes direct numerical simulations and to the classical theory of stretched flames.

Task Significance:

Images of the flame shape and curvature will be used to assess numerical simulations which neglect buoyancy, and to deduce universal, buoyancy free scaling relations showing the effects of vortex size and strength. Understanding of turbulent combustion, applicable to all practical combustion, will be enhanced.

Progress During FY 1996:

The electronics for the spark ignition circuit were received and assembled. Testing was done to determine the proper voltage (8,000 -12,000 volts) to charge the capacitors such that lean mixtures could be ignited and the computer would not be affected. Above 12,000 volts the computer was affected by the spark. The ignition problem was solved by using approximately 10,000 volts and the proper capacitance. Flat and repeatable flames were achieved in the drop rig operated at one-g in our lab. Information was sent to Dr. K. Kailasanth who is developing a direct numerical simulation of our experiment. He solves the exact Navier Stokes equations with complex chemistry for the case a single vortex interacting with a flame of our equivalence ratio. The one-g baseline experimental results have led to some important scientific findings. Strong vortices survive the flame passage and are later strengthened by the flame, which produces additional vorticity as a result of baroclinic torques. Weak vortices are attenuated by the flame but cause the flame to produce additional vortices of opposite sign. These results show that flames create vorticity that significantly affects the flame wrinkling and propagation process. The data is directly useful to certain turbulent flame modellers, such as W. Ashurst at Sandia Labs and D. Haworth at G.M. R&D Center, who have contacted us.

New types of seeding particles were purchased and tested in order to improve our flow visualization and for use as PIV particles. Some aerosil silicon dioxide particles provide better flow seeding than the oil drops that were used previously. The problem that was identified during the July, 1995 2.2 Second Drop Tower drops was that the oil drops evaporated, settled or condensed at the walls during the 20 minute wait time prior to the drop. The silicon dioxide particles should perform much better; testing is still in progress. The repeatability of the flame/vortex experiment was tested with the new modifications. Some additional tests were run to modify the one-g PIV system for use in the 2.2 Second Drop Tower. Light sources were tested and the quality of the images examined. Problems identified during the July 1995 drop tests in the NASA Lewis 2.2 Second Drop Tower Facility have been corrected.

A new sealing system for the exhaust ports was developed and tested. It consists of a thin plastic membrane that covers the exhaust ports. Even with the exhaust ports closed, unwanted air was leaking into the experiment which made the fuel-air mixture too lean to ignite. With the added membrane, the experiment is leak tight. The membrane will be removed just prior a drop. Preparations were made to make some drops in the one second drop facility at the University of Michigan that was built by Professor Herman Merte. It is still necessary to use the NASA 2.2 Second Drop Tower but additional drops at the University of Michigan would allow for a more complete data set. Work continued on developing PIV diagnostics for the drop experiment. Aerosil particles were purchased that remain in suspension, are not consumed by the flame, and yet scatter sufficient light for PIV images. Some electronics and computer equipment required to digitize and analyze the PIV images was researched and the purchase orders submitted.

Most of the non-premixed flame experiment has been assembled by Professor Dahm and J.S. Chen, a graduate student in the department. This experiment is mounted on a drop rig that is separate from the premixed flame experiment. The non-premixed flame experiment consists of a chamber filled with methane that has a mechanical device to force the methane out through a contoured nozzle into a larger chamber that is filled with air. An ignitor is located at the lip of the nozzle. The methane that is force out of the fuel chamber forms a highly repeatable and controllable laminar vortex. The strained nonpremixed flame that exists at the fuel-air boundary will be studied. A light sheet imaging system has been added to the drop rig to visualize the conserved scalar field. A video camera is used to visualize the flame radiation directly and to visualize light scattered from seeding particles. Parts of the DDAC and other electronics were assembled in January but the electronics assembly is not complete.

A series of drops were made at the NASA LeRC 2.2 Second Drop Tower during the week of April 8, 1996. The results of the drop tests are: 1) The amplitude of the wrinkles in the flame caused by the vortex is 1.5 to 2 times larger in microgravity than in the corresponding one-g case, for the same vortex strength, 2) The laminar flame speed (SL) in microgravity is 1.8 times larger than that of the one-g case for a downward propagating flame. This is consistent with observations made that flames moving upward within tubes move significantly faster than those that propagate downward in tubes, 3) Proper comparison requires that both the microgravity and one-g results be compared for the same ratio of vortex strength to laminar burning velocity (U_q/SL). When this parameter is used, microgravity flames have approximately three to four times the amplitude of wrinkling compared to one-g flames, for the same value of U_q/SL . This is a significant difference and suggests that microgravity turbulent flames will wrinkle and propagate faster than corresponding one-g flames, 4) The one-g PIV work provide images of a mechanism that explains why the flames become more wrinkled in microgravity. The PIV images show new vorticity that is created by buoyancy which suppresses the wrinkling in one-g. With this suppression of the wrinkling removed in the microgravity tests, the flames are free to wrinkle. This mechanism is important in explaining turbulent flame results in one-g and should be added to current turbulent combustion models, 5) Flames in microgravity are more curved than one-g flames. This results from the fact that buoyancy forces at one-g tend to flatten the present flame, 6) The microgravity flames appear to have a thicker reaction zone than one-g flames, but further work is required to see if this is real or an artifact of the blurring caused by the video camera shutter time. The microgravity flames move faster so the blurring effect may be larger in the microgravity case, 7) The present experiment provides flames that are stable and wrinkle-free prior to the vortex interaction. The synchronization techniques required to get the flame, vortex, and light sheet in the same place at the correct time during the drop were successful and highly repeatable.

Results from the drop tower tests conducted at NASA Lewis in April 1996 were analyzed and summarized in a abstract that was submitted for the AIAA 35th Aerospace Sciences Meeting to be held in January 1996 in Reno Nevada. This paper is entitled "Flame -Vortex Interactions: Effects of Buoyancy Deduced from Microgravity Imaging Studies", Jose Sinibaldi, Alan Tulkki, Charles Mueller, James F. Driscoll Dept. of Aerospace Engineering, Univ. of Michigan, Ann Arbor, and John Brooker, NASA Lewis Research Center. Results of the microgravity studies to date are as follows: (1) Microgravity conditions greatly enhance the flame wrinkling process in this flame-vortex interaction, as compared to the one-g studies. It can be inferred that fully turbulent flames in microgravity could wrinkle more easily and thus propagate significantly faster than those in one-g, which is a potential safety hazard; (2) A new physical mechanism is identified which explains why microgravity conditions enhance flame wrinkling. PIV measurements at different Froude numbers show that buoyancy retards flame wrinkling; buoyancy produces new vorticity (due to baroclinic torques) that opposes the wrinkling and stretch imposed by the original vortex. Microgravity conditions remove this stabilizing mechanism and therefore the amplitude of flame wrinkling is found to increase by a factor of 3-4; (3) Buoyancy forces are found to cause an increase in the flame speed. It is believed that buoyancy forces cause the hot products to remain in closer contact

with the reaction zone, which enhances the reaction; (4) The results indicate that it is important add buoyancy terms to models of turbulent flames in order to correctly use the models to predict the turbulent burning velocity. The burning velocity depends on the flame wrinkling and flame stretch which is affected by buoyancy in many cases.

Professor Dahm's experiment was built and tested at one-g in preparation for August 1996 drops at the NASA Lewis 2.2 Second Drop Tower. The experiment provides a unique way to study the interaction of a vortex and a non-premixed flame. Methods to properly ignite the flame were tested and the vortex strength was measured and calibrated. Certain safety aspects of the experiment were considered since fuel for several drops is carried on the package. Analysis and tests were conducted in order to optimize safety and to eliminate potential problems.

Sixteen drops of the University of Michigan Flame-Vortex Interaction Experiment (premixed) were made during the week of August 19th at the NASA Lewis 2.2 Second Drop Tower. Useful measurements were obtained on 50% of the drops. On the other 50% of the drops, the new conditions created by microgravity caused some problems that can be eliminated on future drops. The impact caused by the drop caused the loudspeaker to malfunction on the subsequent drop in some cases. However the success rate of 50% is considered to be adequate. A new fuel type (methane) was used for the August 1996 drops, which replaced the fuel (propane) used in our previous drops. The new fuel has different thermo-diffusive characteristics and creates a new instability in the flame. It was found that the flame wrinkles more easily with methane as expected. Analysis of the drop tower data is in progress. The non-premixed flame experiment of Professor Dahm was brought to NASA Lewis for a safety inspection and for preparation for a series of drops in the 2.2 Second Drop Tower.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 5/94 EXPIRATION: 4/98

PROJECT IDENTIFICATION: 962-22-05-45

NASA CONTRACT No.: NAG3-163

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Mueller, C.J., Driscoll, J.F., Reuss, D.L., Drake, M.C., and Rosalik, M.E., Generation and attenuation of vorticity by flames: measured vorticity field time evolution during a premixed flame-vortex interaction. Combustion & Flame, (in print 1996).

*Aerodynamic, Unsteady, Kinetic, and Heat Loss Effects on the Dynamics and Structure of Weakly-Burning Flames in Microgravity***PRINCIPAL INVESTIGATOR:** Prof. Fokion N. Egolfopoulos

University of Southern California

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

To obtain quantitative information (flame speed, velocity field, temperature) about the characteristics of weakly burning flames in microgravity, and to use this information to analyze near-limit phenomena at normal gravity conditions.

Task Description:

The experiments will employ a counter-flow burner geometry to provide a nearly adiabatic flame with well controlled strain, for conditions that cannot be achieved in normal gravity. Both premixed and diffusion flames will be studied at various pressures, and Laser Doppler Velocimetry, Particle Image Velocimetry and high-speed cinematography will be used to measure the flow fields. Models will be developed for these cases for comparison purposes. In addition, flame interactions will be studied, and numerical simulations of flame propagation in tubes in spherical vessels will be performed. Experiments will be conducted at normal gravity, in the 2.2 Second Drop Tower, and aboard the DC-9 aircraft.

Task Significance:

The research will allow for the first time a study of flames burning near their flammability limit (the concentration of fuel in air that just forms a flammable mixture) without the complications of buoyancy, wall heat losses or time-varying strain. It will provide fundamental data about the flammability limits that can be used to verify theoretical calculations, and has applications to turbulent combustion such as that found in engines.

Progress During FY 1996:

Work this year was directed towards measuring the flow field in the region upstream of the flame. A particle seeder developed at NASA Lewis was installed on the rig and a series of drops were conducted to visualize the gas flow as it exited the burner. We obtained qualitative images of flow patterns. Unfortunately, a series of problems arose which prevented us from obtaining quantitative data via Particle Image Velocimetry (PIV). The main shortcoming was the laser diode we installed on the rig which did not provide sufficient light intensity to reliably track the particles. We are in the process of mounting optics on the rig that will form a light sheet from a more powerful laser that will be mounted at the top of the drop tower and routed to the drop rig via a fiber optic cable. High-speed video is also being considered as a way to improve the visualization. We also had problems with the screens in the burners getting clogged that caused ignition problems, as well as some mixing deficiencies; both of these issues have been resolved.

In order to simplify the burner arrangement, the upper burner was removed and replaced with a flat plate to yield a stagnation flame. The distance between the plate and the lower burner is variable so that it can be moved during the drop to vary the strain to determine the extinction strain rate. During testing it was recognized that the flame could be stabilized beneath the plate either as a stagnation flame (positively strained), or, for low-enough flow rates or high enough plate separations, as a Bunsen flame (negatively strained). Between these two regimes it is now hypothesized that there is a region where the strain rate is zero. It is our goal to stabilize the flame at that flow rate/plate separation in 0-g to obtain a true zero-strain flame.

A study was undertaken of the flame instabilities for the stagnation geometry, in particular the traveling waves that appear at low strain rates. Experiments were conducted at 1-g to determine flame speeds at the lowest possible strain rates below which instabilities appear. In addition previously unreported flame instabilities at high strain rates were also detected. LDV was used to measure the centerline velocity, and tests were conducted for strain rates from near zero to 50 1/s. This data will complement the microgravity data expected to be obtained on the next visit to NASA Lewis.

Also, experiments were begun on flames with an unsteady imposed strain rate, using an acoustic speaker to modulate the flow. Tests were conducted using methane air mixtures and graphs were generated showing the flame displacement vs. frequency of imposed strain rate. As predicted by a previously developed theory, attenuation of the flame oscillation is obtained for values of the Stokes parameter greater than one ($(w/2K_{\text{mean}})^{1/2} > 1$).

A major upgrade of the numerical model commenced in which the calculations now account for variations in the r-direction for the stagnation flow, rather than assuming conditions that only vary in one dimension along the stagnation streamline. Initial testing of the code using hydrogen, which has fewer reactions to consider, has begun.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 5/94 EXPIRATION: 4/98

PROJECT IDENTIFICATION: 962-22-05-50

NASA CONTRACT NO.: NAG3-161

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Egolfopoulos, F.N., Zhang, H. and Zhang, Z., Wall effects on the propagation and extinction of strained, laminar, premixed flames. Combustion and Flame, (to appear, 1996).

Presentations

Egolfopoulos, F.N., Zhang, H., Vagelopoulos, C.M., and Zhang, Z. "Dynamic and stability effects on counterflowing laminar premixed flames: Implications on the determination of laminar flame speeds." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28-August 2, 1996.

Egolfopoulos, F.N., Zhang, H., Zhang, Z., and Kastanas, G., "Wall effects on the propagation and extinction of strained, laminar, premixed flames." Fall Meeting, Western States Section of the Combustion Institute, Stanford University, Palo Alto, California, Paper No. 95F-215, October 30-31, 1995.

Detailed Studies on the Structure and Dynamics of Reacting Dusty Flows at Normal and Microgravity

PRINCIPAL INVESTIGATOR: Prof. Fokion N. Egolfopoulos

University of Southern California

CO-INVESTIGATORS:

Campbell, C.S.

University of Southern California

Task Objective:

To obtain measurements of the structure and response of lightly loaded dusty gas mixtures (using both combustible and inert particles) in a simple counterflow flame environment under both normal- and micro-gravity conditions. The primary goal is to investigate the effects of the inertially imposed inability of the particles to follow the gas flowfield. The results will be compared to a concurrently developed theoretical model.

Task Description:

The counterflow environment in which the experiments will be conducted and which will be theoretically analyzed has several advantages for this type of study; in particular, it provides a simple strained gas flow-field that will be difficult for particles, especially large particles, to follow exactly. A phased Doppler anemometer will be used to independently track the particle and gas velocities and the particle size (which may change during burning) and particle concentration; this will provide enough detailed information to be compared against the theoretical predictions. Inert particles will be examined first to observe the effects of the added heat capacity on premixed flames. Tests on combustible particles will follow. Experiments will be performed in normal gravity, in the 2.2 Second Drop Tower and aboard the DC-9 aircraft.

Task Significance:

Particle-laden combustible mixtures are an integral part of many industrial hazards. Conditions leading to their flammability are not well understood, in part because gravity forces particles to settle out of a gas flow. Thus, at normal gravity both gravity and the particle inertia cause a non-convergence of the particle and gas flowfields. This can be a particular problem for large particles and low velocity gas flows for which gravity may dominate the hydrodynamic effects. Performing the experiments in micro-gravity allows the gravitational settling to be eliminated leaving only the hydrodynamic effects. Comparison between the micro- and normal- gravity results will allow gravitational effects to be understood. These will be the first tests that permit such a distinction to be made.

Progress During FY 1996:

This is a new grant which was just initiated June 1996.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-22-00

NASA CONTRACT No.: NAG3-187

RESPONSIBLE CENTER: LeRC

Effects of Gravity on Sheared and Nonsheared Turbulent Nonpremixed Flames

PRINCIPAL INVESTIGATOR: Prof. Said E. Elghobashi

University of California, Irvine

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The task objective is to answer fundamental questions regarding the effect of buoyancy on turbulent combustion. These questions include:

- 1) How does buoyancy affect the small-scale structure of the scalar and velocity fields?
- 2) How does buoyancy affect the distribution of scalar dissipation near the reaction zone?
- 3) Is the flamelet model valid for buoyant turbulent diffusion flames?
- 4) How does flame extinction depend on the appropriate non-dimensional numbers (Fr , Da , Re , etc.), the magnitude of the reaction energy, and the direction of gravity relative to the fuel-air interface?

Task Description:

This research is entirely computational. It will focus on direct numerical simulation (DNS) of two cases of flow: an initially-homogeneous turbulent flow without shear, and a flow with initially uniform shear. In both cases separate, parallel streams of fuel and oxidizer will enter the computational domain and react. Numerical models that have already been developed by the Principal Investigator will be extended to these cases with principal additions to include finite rate chemistry and non-zero gravity. The results will be presented in the form of diagrams based on the appropriate nondimensional numbers.

Task Significance:

This work will answer fundamental questions about how buoyancy induced by gravity affects turbulent combustion. In particular, gas, temperature, and velocity distributions can be very different without the flows caused by gravity, and this research will focus on revealing the small-scale structural differences in the flame, as well as probing the dependence of flame extinction on the alignment between gravity and the fuel-air interface. With this information, mathematical models of turbulent diffusion flames can be modified to better account for buoyancy effects. Better understanding of the physical processes will lead to improved combustor design and enhanced predictive capabilities regarding fires on Earth and in a space environment.

Progress During FY 1996:

Some of our effort during the past year was concentrated on performing detailed analysis of the infinite-rate reaction flow with and without buoyancy. We found that both for the buoyant and non-buoyant cases, strain dominates the flow field (i.e. on the average the strain values are much larger than those of enstrophy or velocity divergence square.) We also focused on the influence of buoyancy on the pdf's of the mixture fraction and its dissipation. We found that as a result of buoyancy, the fluid is transported from the lower (oxidant) to upper (fuel) side and high dissipation of mixture fraction values do not coincide with the reaction zone. We found that the dissipation of temperature to be the quantity which coincides with the reaction zone perfectly.

In addition, we began simulations of the finite reaction-rate case with Damkohler numbers from 1000 to 5000 and started investigating the physics in this flow. We have observed that the reaction rate is a function of scalar dissipation and the mixture fraction in these flows. Based on this observation, we have developed a modified flamelet model. We computed the reaction rate based on this model and compared it with DNS results. Correlations between reaction rate, mixture fraction, temperature, and vorticity were obtained for finite Damkohler number ($Da=1000$ and 5000) runs for the buoyant case. We superposed two (or three) of these variables on contour plots to examine their correlations.

Lastly, work was started on the effect of changing the gravity direction relative to the interface between the fuel and oxidant streams. In all previous cases the gravity vector was perpendicular to the interface (e.g. a horizontal flame). Now, we are examining the case where the gravity vector is parallel to the interface (e.g. a vertical flame). We modified the boundary conditions in our code to simulate a vertical flame under different gravity magnitudes. In order to insure that the results are not sensitive to the conditions at the outflow boundary we increased the length of the domain in the gravity direction. For the horizontal flames that we studied earlier we used a cubic domain. Particular focus is given to the modification of the pressure solver. We considered the case when the grid spacing in all three directions is the same, but the number of points are different. We performed test runs for the horizontal flame to investigate whether the aspect ratio of the domain has any influence on the results.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 5/94 EXPIRATION: 5/98

PROJECT IDENTIFICATION: 962-22-05-59

NASA CONTRACT NO.: NAG3-160

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Boratav, O., Elghobashi, S., and Zhong, R., On the alignment of alpha-strain and vorticity in nonpremixed flames. Physics of Fluids, vol. 8 (8), 2251-2253 (August 1996).

Elghobashi, S., Boratav, O.N., and Zhong, R., Effects of buoyancy on turbulent nonpremixed flames. Bulletin of APS, vol. 40 (12), 1991 (October 1995).

Proceedings

Boratav, O., Elghobashi, S., and Zhong, R., "Buoyancy effects on the structure of turbulence in nonpremixed flames." Proceedings of the SIAM - 6th International Conference on Numerical Combustion, New Orleans, March 4-6, 1996.

Presentations

Elghobashi, S., Boratav, O. and Zhong, R., "Effects of buoyancy on turbulent nonpremixed flames." Invited lecture at the International Conference on Turbulent Heat Transfer, San Diego, March 10-15, 1996.

Soot Processes in Freely-Propagating Laminar Premixed Flames

PRINCIPAL INVESTIGATOR: Prof. Gerard M. Faeth

University of Michigan

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This ground-based project is an experimental and theoretical investigation of soot formation in laminar freely-propagating premixed flames under conditions of low buoyancy. The ground experiment uses a free-fall system developed at the Gas Dynamics Laboratories of The University of Michigan.

Task Description:

Experiments will address several aspects of freely-propagating laminar premixed flames while emphasizing soot processes in hydrocarbon-fueled flames. The experiments involve premixed flames that are spark-ignited at the center of a spherical windowed chamber in free-fall in a short-drop (roughly 1 m) facility with reactant mixtures initially at room temperature and pressures in the range 0.2-3.0 atm. Reactants involve hydrocarbon fuels having various H/C ratios and burning in either air or oxygen-enriched air. Measurements include the following: deconvoluted laser extinction for soot concentrations, deconvoluted multiline emission for soot temperatures, thermophoretic sampling and analysis by transmission electron microscopy (TEM) for soot structure, sampling and analysis by gas chromatography for the concentrations of major gas species, particle-image velocimetry (PIV) for gas velocities, and schlieren motion picture photography for flame positions (or rate of propagation). Analysis includes numerical simulations based on detailed chemical mechanisms to predict the structure of both the flame and post-flame regions as well as hydrocarbon-abstraction/carbon-addition (HACA) mechanisms of soot growth.

Task Significance:

In most flames of practical interest, soot radiation is the dominant mode of heat transport to combustor components and a dominant mechanism for flame spread and growth while soot emissions are a dominant mode of particulate, unburned hydrocarbon (including polyaromatic hydrocarbons or PAH) and carbon monoxide emissions. The experimental results, combined with theoretical modeling, will increase our fundamental understanding of soot formation processes in both laminar and turbulent flames as well as our abilities to model these processes. A most important advance of the present work involves results at elevated pressures where exploitation of low gravity provides a way to complete detailed measurements that are not feasible on earth due to the intrusion of buoyancy. Consequently, the results of the investigation will have a significant impact on our understanding of processes and systems such as the spread of unwanted fires, the design of jet engines and gas turbine power systems, the design of diesel engines and the design of large-scale boilers, among others.

Progress During FY 1996:

The progress in this year includes completion of design of the test apparatus; fabrication of the test chamber, and assembly of the gas supply and ignition systems. The new apparatus will be constructed of stainless-steel welding caps with quartz windows.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 7/96 EXPIRATION: 7/00

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NAG3-187

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Lin, K-C., Sunderland, P.B., and Faeth, G.M., Soot nucleation and growth in laminar acetylene/air diffusion flames. Combustion and Flame, (1996).

Proceedings

Faeth, G.M. and Koylu, U.O., "Structure and optical properties of flame-generated soot." Proceedings of the 8th International Symposium on Transport Phenomena in Combustion. November, 1995.

Combustion of Electrostatic Sprays of Liquid Fuels in Laminar and Turbulent Regimes

PRINCIPAL INVESTIGATOR: Prof. Alessandro Gomez

Yale University

CO-INVESTIGATORS:

Long, M.B.

Yale University

Smooke, M.D.

Yale University

Task Objective:

The focus of this project is the study of the formation and burning of sprays of liquid fuels at both normal and reduced gravity. The objective is to synthesize gradually the complexity of practical combustion systems, using well-defined sprays to generate controlled clouds of droplets to be burned in well-characterized combustion environments.

Task Description:

The program is strategically articulated in three parts: an experimental one at normal gravity, in the combustion laboratories at Yale; an experimental part at reduced gravity, in the 2.2s drop tower at NASA-Lewis, and a computational part that parallels the experimental components. The microgravity experiments are aimed at studying the same types of sprays that have been previously examined at normal gravity in an environment free of natural convection effects. The numerical modeling is pursued to facilitate the interpretation of the experimental results and to complement the measurements, especially in the microgravity phase of the project, in which the constraints on available diagnostic techniques are severe.

Electrostatic sprays and ultrasonic nebulizers are used as atomizers. Experiments are conducted first in counterflow and co-flow laminar diffusion flames.

Task Significance:

This project should lead to an improved understanding of spray combustion which might ultimately lead to improvements in the practical implementation of liquid fuel atomization, for example in diesel or liquid-fueled rocket engines.

Progress During FY 1996:Coflow Laminar Spray Diffusion Flames

We completed the study of an axisymmetric co-flow spray diffusion flames, using an electrospray as an atomizer source. We showed an unparalleled level of control in the spray burning mode that was achieved by simply varying the feed stream composition. Two flames were stabilized at constant injector conditions, that is, without changing fuel flow rate or applied voltage between the electrodes. Such conditions corresponded to the generation of monodisperse and electrically-charged droplets with mean diameter of 52 micro-m. The first flame had a candle-like appearance. We will refer to it as the base case flame. Rather than burning, the majority of the droplets simply evaporated at low temperatures in the inner core of the flame, which appeared as a relatively dark region. This inner core was enveloped by a higher temperature region where soot was present. Outside of the sooty region, a flame characterized by a soft blue luminescence could be clearly seen in the lower half of the luminous combustion region. The flame was lifted off the burner by the distance (few millimeters) required to vaporize enough fuel to establish a premixed stabilizing ring flame. Quantitative measurements of interdroplets distance and droplet group combustion number showed that the base case flame burned in an *internal or partial* group combustion mode, with the bulk of the droplets surrounded by a common flame and only a few of them burning outside as individual droplets. Decreasing that flame group combustion number by decreasing the flame radius via oxygen enrichment of the oxidizer stream was shown to cause an increase of the fraction of droplets burning individually outside the flame core. At a molar oxygen concentration and 0.62 in the oxidizer stream, the transition to individual droplet burning was complete, as manifested by the flame appearance as a collection of chemiluminescent streaks radiating from a common origin. This is the first experimental system that allows for a good control of the spray group burning mode and the continuous monitoring of the transition from one burning regime to another. An article on this subject is currently under review in *Combust. Flame*.

Relying on a source of virtually monodisperse droplets offered unique advantages in the implementation of diagnostic techniques and in the interpretation of the results. The extraction of information on the droplet evaporation behavior, such as an evaporation coefficient becomes relatively trivial, once droplet size and velocity are simultaneously measured. In the cited reference in *Combust. Sci. and Tech.* we showed that in the base case flame, despite the evidence of internal group combustion mode, droplet interaction was not sufficiently intense to cause a departure from d-square law. A comparison of the droplet evaporation time to a characteristic diffusion time showed that the latter is much longer, which implies that these spray flames are still diffusion-controlled. Experiments under microgravity conditions in the Drop Tower showed that the flames are longer, wider and brighter than the normal-gravity counterparts, which can be attributed to an increase in residence time in the flames as buoyant acceleration of the gas is diminished. Measurements of the gas velocity field on the axis of the flame showed that the flame was under a mixed regime, with a momentum-controlled lower part and a buoyancy-controlled upper region.

Counterflow Laminar Spray Diffusion Flames

We completed a comprehensive numerical model for laminar counterflow spray diffusion flames, using detailed chemical kinetics and transport, and sectional conservation equations to follow the evolution of the droplet size distribution, as further elaborated in the presentation at the *26th International Symposium on Combustion*. The steady-state, two-dimensional axisymmetric governing equations for the conservation of mass, chemical species, momentum and energy in the gas-phase were modified to include source/sink contributions accounting for the interaction with the fuel droplets. The statistical droplet size distribution, that had been experimentally measured by a Phase Doppler technique, was discretized into a number of sections. For each section, conservation equations were specified for mass, momentum and energy that enabled us to compute the source/sink terms in the gas-phase governing equations, through which the two phases were coupled. The complexity of the system of gas equations was reduced by seeking a similarity solution, that, when substituted into the two-dimensional governing equations, yielded a nonlinear two-point boundary value problem in the axial direction.

In the presence of a spray, such similarity solutions could only be derived under some restrictive assumptions on the liquid phase. Specifically, the model is limited to small slip velocities or small droplet Reynolds numbers, a condition that cannot be fulfilled using an electrospray. Thus, a commercial ultrasonic nebulizer was coupled to our burner. Since droplets are generated gently by vibrating a piezoelectric crystal at ultrasonic frequencies, they are dragged into the combustion environment by the host flow under conditions of modest slip. Experimental measurements provided the boundary conditions for the numerical code.

It was found that for *quantitative* comparison between experiments and calculations it was necessary that the velocity gradient at the boundary be carefully determined, without relying on a priori assumptions on the type of (plug versus potential) flow. Under such conditions, the agreement between gas-phase temperature measurements and computations was excellent. Good agreement between experiments and calculations was also found in droplet size distribution along the axis of the flame, which shows that the droplet vaporization behavior is correctly represented. In the present flame no *direct* interaction between droplets and flame exist. Rather, after the droplets evaporate, the fuel vapor diffuses and/or is convected into the flame, as in ordinary gaseous diffusion flames. Although the present emphasis was not on the influence of liquid fuel dispersion on chemical species in flames, the successful validation of the code with respect to the physical variables suggests that it is capable of addressing this issue, especially in the context of pollutant formation.

Diagnostics Techniques

Although our emphasis has been to study combustion aspects using available diagnostics, at times we had to develop diagnostic tools. Two projects were developed in this context: one was aimed at measuring droplet size with accuracy greater than that of Phase Doppler interferometric techniques; the other focused on the measurement of gas-phase temperature in turbulent spray flames. On the first subject, the need for such method stems from the fact that Phase Doppler has a reported accuracy of 4% in size that translates into 12% in volume. Clearly, quantification of droplet evaporation rates necessitate size measurements with improved resolution. We developed a technique that entails imaging on a photodiode array the angular scattering intensity collected by a lens and applying a Fast Fourier Transform (FFT) to the array serial output to recover an effective frequency and phase corresponding to the number and position of the scattering lobes. The method yields the determination of size with an accuracy better than 1%, if the index of refraction is known and constant. The technique can be in principle applied at data rates as high as tens of KHz with modest equipment investment, which makes it well-suited for the measurement of droplet evaporation

rates in dilute sprays in real time. Errors associated with particle trajectory effects and changes in the index of refraction were also considered, as further elaborated in the cited reference in *Applied Optics*.

Before we embarked in a detailed characterization of turbulent spray flames, we needed to identify a means to measure temperature probability density function. To this end, we developed a single point Stokes/Antistokes spontaneous Raman thermometry technique and demonstrated the feasibility of measuring the ensemble probability density function (pdf) of the gas-phase temperature in a spray flame. Using optical and acoustic techniques, interference effects from laser induced breakdown, droplet elastics light scattering and fluorescence were successfully screened out. The technique yields single point measurements of the ensemble probability density function (pdf) of the gas-phase temperature in a spray flame, as documented in the cited reference in *Optics Letters*. It is currently being applied in a newly developed turbulent spray flame and supplemented by Phase Doppler interferometric techniques.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 3/91 EXPIRATION: 12/98

PROJECT IDENTIFICATION: 962-22-05-34

NASA CONTRACT NO.: NAG3-168

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Chen, G. and Gomez, A., Co-flow laminar diffusion flames of monodisperse sprays: structure, evaporation and microgravity effects. *Combust. Sci. and Tech.*, 115, p. 199 (1996).

Karpetis, A. N. and Gomez, A., Temperature measurements in spray flames using spontaneous raman scattering. *Optics Letters*, 21, p. 704 (1996).

Min, S. and Gomez, A. High resolution measurement of single spherical particles using the FFT of the angular scattering intensity. *Applied Optics*, (August, 1996).

Proceedings

Chen, G. and Gomez, A., "Group combustion of a dilute spray in a co-flow laminar diffusion flame." *Proceedings of the Third Asian-Pacific International Symposium on Combustion and Energy Utilization*, Hong Kong, vol. 2, p. 384, December 11-15, 1995.

Books

Chen, G. and Gomez, A., "Recent Advances in Spray Combustion, Chapter Title: The structure of a co-flow laminar diffusion flame." Edited by: K.Kuo, Ed AIAA Book Series, October 1995.

Presentations

Chen, G. and Gomez, A. "Group combustion in co-flow laminar diffusion flame." presented at the 1995 Technical meeting Eastern States Section of the Combustion Institute, Worcester, MA, October 1995.

Chen, G. and Gomez, A., "Co-flow laminar diffusion flames of monodisperse sprays: structure, group combustion and microgravity effects." Paper 95-F70 presented at the 1995 Fall Meeting of the Western States Section/The Combustion Institute, Stanford CA, October 1995.

D'Angelo, Y., Silverman, I., Gao, L.P., Gomez, A. and Smooke, M.D., "Computational and experimental study of counterflow spray diffusion flames." presented at the 1995 Technical Meeting of the Eastern States Section / The Combustion Institute, Worcester, MA, October 1995.

Gao, L.P., D'Angelo, Y., Silverman, I., Gomez, A. and Smooke, M.D., "Quantitative comparison of detailed numerical computations and experiments in counterflow spray diffusion flames." Paper presented at the Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28 to August 2, 1996.

Karpetis, A. N. and Gomez, A., "Gas temperature measurements by Stokes/Anti-Stokes raman thermometry in spray flames." presented at the 1995 Technical Meeting of the Eastern States Section / The Combustion Institute, Worcester, MA, October 1995.

Characteristics of Non-Premixed Turbulent Flames in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Uday Hegde

NYMA, Inc.

CO-INVESTIGATORS:

Stocker, D.
Bahadori, M.Y.NASA Lewis Research Center (LeRC)
Science Applications International Corporation

Task Objective:

The overall objectives of this project are:

1. To obtain and analyze experimental data on flame images, and spatial and temporal distributions of velocity, temperature, radiation, and gas species in microgravity turbulent gas-jet diffusion flames and
2. To validate and refine existing predictive capabilities.

Task Description:

A series of ground-based tests in the NASA Lewis reduced gravity facilities i.e., the 2.2 Second Drop Tower, the Zero-G Facility and the DC-9 aircraft will be conducted to elucidate the behavior of turbulent non-premixed flames in low gravity. Pertinent experimental data including flame shape and size, temperature and velocity will be compared with the results of numerical modelling.

Task Significance:

The proposed research has value from both fundamental and practical viewpoints. It will improve fundamental understanding of turbulence characteristics in gas-jet diffusion flames not only under microgravity conditions but also under momentum-dominated conditions on earth. This understanding has a wide range of practical applications such as diffusion flames in industrial combustors where, because of high velocities, buoyancy effects are small, and in the turbulence decay process in large-scale fires. Studies of momentum-dominated flames in normal gravity require large jet velocities which leads to difficulties in resolving the smaller scales of the turbulent motion thereby precluding an in-depth understanding of the flame characteristics. In a microgravity environment, the jet velocity can be reduced while still maintaining both turbulent and momentum-dominated conditions and the smaller scales can be resolved.

Progress During FY 1996:

The task commenced in June 1996.

The test matrix for the 2.2 Second Drop Tower tests has been developed. A series of tests will be conducted in the drop tower to select the flames to be studied in the Zero-G Facility and the DC-9 aircraft. The drop rig has been designed and assembly has begun. It is expected to be completed by January 1997, at which time drop testing will commence.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-22-05

NASA CONTRACT NO.: NAS3-960

RESPONSIBLE CENTER: LeRC

Three-Dimensional Flow in a Microgravity Diffusion Flame

PRINCIPAL INVESTIGATOR: Prof. Jean R. Hertzberg

University of Colorado, Boulder

CO-INVESTIGATORS:

Linne, M.A.

Colorado School of Mines

Task Objective:

The objective is to study the influence of buoyancy on the three-dimensional fluid dynamics of the interaction between a diffusion flame and the elliptic vortex rings formed by pulsations of the fuel flow issuing from an elliptic nozzle.

Task Description:

A methane diffusion flame burning in atmospheric conditions is investigated. Elliptic vortex rings are generated by a combination of periodic flow perturbations (active forcing) and the elliptic geometry of the fuel nozzle (passive forcing). The fuel flow is forced by an in-line 100 watt loudspeaker system at frequencies up to 1 KHz. Phase-locked flow visualization and particle image velocimetry (PIV) are the primary diagnostics.

Task Significance:

Techniques of active and passive control of the fluid dynamics in diffusion flames have the potential to enhance combustion efficiency and reduce pollutant formation. Potential applications include industrial and residential burners and gas/liquid fueled engines.

Progress During FY 1996:

Entrainment and mixing in isothermal jets are easily controlled by active and passive forcing techniques. However, jet diffusion flames are more difficult to control for several reasons: both hydrogen and hydrocarbon flames form on the outer edges of the shear layer region and the effects of heat release (with the exception of buoyancy) act to stabilize the flow. However, under specific active forcing conditions in the absence of coflow, a large scale, global change in flame behavior can be induced. The flame becomes shorter, blue in color, and 'split' into a central jet and one or two side jets. Depending on the forcing level, the behavior bifurcates in time, switching between a classical diffusion flame and the split flame. This suggests that the flame can intermittently suppress the instability responsible for the split fuel jet.

This behavior has been observed in two combustors; one a fully axisymmetric configuration with a tube nozzle, and a combustor with a rectangular plenum and an elliptic cross section nozzle which exits through a flat plate. The latter combustor has been designed for normal, inverted and microgravity conditions. A coflowing air stream as is customary in jet diffusion flame experiments is not used due to difficulties in the inverted position; hence the flat plate boundary condition is used instead. The split flame behavior has been observed at frequencies roughly corresponding to peaks in the acoustic response of each combustor. In the case of the microgravity combustor, splitting behavior has been observed at up to 800 Hz.

Scoping studies and flow visualization in normal and inverted gravity have been carried out. In normal gravity, the elliptic nozzle causes four side jets to form, as shown by laser sheet visualization. Side jets form along the major axis by 3 mm downstream, and along the minor axis by 19 mm. With appropriate shielding, the elliptic nozzle partially stabilizes the azimuthal wandering of the side jets, allowing vertical views to be studied, although generally only a single side jet is visible at a time. The vertical cuts show a secondary vortex structure developing on top of the primary vortex ring which seems to be related to the development of the side jet. This has not been observed in other studies of side jets. The horizontal cuts reveal an extremely complex three-dimensional structure in which the bilateral symmetry of the nozzle exit is preserved for only a short distance downstream. Thus vertical cuts of this flow field must be carefully interpreted, and a tomographic reconstruction of the flow from a series of phase locked horizontal cuts will be required to understand the detailed vortex dynamics.

The reacting split jet has a topography similar to the non-reacting jet with several major differences. The flame splits primarily along the minor axis, and only one side jet flame is observed; however, horizontal sheet

visualization has not been performed. The non-reacting jet splits under a wide range of conditions, while the flame splits under higher levels of excitation. Preliminary tests under inverted gravity show no evidence of splitting in either the reacting or non reacting jet, although full scoping studies are not yet complete. This data suggests that buoyancy plays a role in the development of side jets for our conditions. However, the flow is extremely unstable under inverted gravity, and other effects such as the entrainment of jet fluid due to downstream flow reversal may affect the splitting phenomenon.

Prior to carrying out Particle Image Velocimetry (PIV) on this flow, a study has been made of how uncertainties in the velocity field propagate through to the calculation of vorticity fields. A synthetic velocity field was generated from a prescribed vorticity field, and specific errors approximating those of real PIV data uncertainties were introduced. The vorticity field was then calculated from the error laden velocity data at several stages in the post-processing smoothing procedure, and the actual error in vorticity was calculated. Both cross-correlated and autocorrelated PIV were evaluated. The smallest errors were produced with a technique that combines a local regression technique with a cubic spline routine and a Gaussian smoothing mask. The velocity field is repeatedly passed through this procedure until the calculation of vorticity by Stokes' line integral (determined by 'good' unsmoothed vectors only) and area integrals of vorticity agree when compared over a large domain.

Plans include preliminary drop tower tests at the Colorado School of Mines, followed by drop tests in the Lewis 2.2 second tower. Normal and inverted gravity PIV studies are underway as well.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/94 EXPIRATION: 5/98

PROJECT IDENTIFICATION: 962-22-05-58

NASA CONTRACT NO.: NAG3-161

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Hertzberg, J.R., Conditions for a split diffusion flame. Combustion and Flame, (in press).

Luff, J.D., Rompage, A.M., Linne, M.A., and Hertzberg, J.R., Uncertainties associated with the post-processing of 2-D particle imaging velocimetry (PIV) velocity data of unsteady flow fields. Experiments in Fluids, (in press).

Books

Luff, J., "Uncertainties associated with the post-processing of 2-D particle imaging velocimetry (PIV) velocity data in unsteady flow fields." Colorado School of Mines thesis no. T-4831, November 1995.

Presentations

Hertzberg, J., Carlton, J., Bradley, E., Luff, J., and Linne, M., "A split, bifurcated diffusion flame." Presentation HF5 at the 48th Annual Division of Fluid Dynamics, American Physical Society Meeting, November 19-21, Irvine, CA. Abstract published in Bull. APS Volume 40, no. 12, pp. 2015, October 1995.

Hertzberg, J., Carlton, J., Schweiterman, M., Bradley, L., and Linne M., "Splitting of an axially excited jet diffusion flame." Work-In-Progress Poster 2-017 at the 26th International Symposium on Combustion, Naples, Italy, July 29-August 2, 1996.

Luff, J.D., Rompage, A.M., Linne, M.A., and Hertzberg, J.R., "Uncertainties associated with the post-processing of 2-D particle image velocimetry (PIV) velocity data of unsteady flow fields." Paper Number WSS 96S-005, Spring Meeting Western States Section / the Combustion Institute, Tempe, AZ, March, 1996.

Luff, J.D., Rompage, A.M., Linne, M.A., and Hertzberg, J.R., "Uncertainties associated with the post-processing of (PIV) data." Work-In-Progress Poster 5-017 at the 26th International Symposium on Combustion, Naples, Italy, July 29-August 2, 1996.

Combustion Synthesis of Fullerenes and Fullerenic Nanostructures in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Jack B. Howard

Massachusetts Institute of Technology (MIT)

CO-INVESTIGATORS:

Brooker, J.E.

NASA Lewis Research Center (LeRC)

Task Objective:

The objectives of this research are to determine the effects of gravity on fullerene formation in flames and, based on the observed effects, to develop fundamental understanding of fullerene formation and to identify engineering principles for fullerene production.

Task Description:

Fullerenes, the recently discovered form of carbon, consist of closed cages or shells and include molecules of various sizes, from spherical C₆₀ and elliptical C₇₀ to giant fullerenes and nanostructures. The understanding of fullerene formation in flames is at an early stage where there is much need for basic information to be provided by combustion research. The method consists of the operation of laminar premixed and diffusion flames under normal and reduced gravity in a sub-atmospheric combustion chamber, followed by collection of condensibles including soot, polycyclic aromatic hydrocarbons and any fullerenes present within the flame.

Task Significance:

The significance of the expected results will be a better understanding of the types and yields of fullerenes that can be synthesized in flames and the mechanisms of their formation. This information will clarify the chemistry of fullerene formation and the potential for large scale production of different types of fullerenes. Also, fullerene formation in flames has significant similarity to soot formation in that molecular weight growth reactions involving polycyclic aromatic hydrocarbons and acetylene appear to be important in both cases. Therefore, this research can be expected to improve the understanding of formation chemistry of soot as well as fullerenes.

Progress During FY 1996:

A meeting between Prof. Jack Howard, Dr. Henning Richter, Bill Grieco, and John Brooker was conducted at MIT to discuss the fullerenes research project. A decision was made to use toluene as the fuel. Vaporization will occur by directly heating the liquid fuel supply bottle with heat tape and delivering the vapor with a heated vapor source flow controller. Design of the data acquisition and control system is complete and equipment has been ordered. Design and fabrication of the fuel delivery system is in progress.

Effort continues to design and fabricate a data acquisition and control system for use on the DC-9 Reduced Gravity Aircraft. A method to deliver a constant flow of toluene vapor to the combustion chamber has not been determined, however, the use of a syringe pump and an evaporator is the prime candidate since vapor source mass flow controllers are not able to achieve the full range of flow rates.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-22-05

NASA CONTRACT NO.: NAG3-187

RESPONSIBLE CENTER: LeRC

Unsteady Numerical Simulations of the Stability and Dynamics of Flames in Microgravity

PRINCIPAL INVESTIGATOR: Dr. K. Kailasanath

Naval Research Laboratory (NRL)

CO-INVESTIGATORS:

Patnaik, G.
Oran, E.S.

Berkeley Research Associates
Naval Research Labs

Task Objective:

The objective is to study the structure (multidimensional) and dynamics (propagation, stability and extinction) of premixed flames in micro- and normal-gravity environments.

Task Description:

The task involves performing detailed numerical simulations using time-dependent, one-, two- and three-dimensional flame models. These models solve the multispecies coupled partial differential reactive-flow equations, including fluid, thermodynamic and transport properties, chemical kinetics, radiative heat transfer, buoyancy and boundary heat loss effects. The investigator will a) systematically isolate and evaluate the relative importance of various physical and chemical processes that may be controlling the structure and dynamics of premixed flames, and b) compare qualitatively and quantitatively with experimental observations.

Task Significance:

Small amounts of fuel leaking from fuel cells could pose a fire hazard on the space-shuttle and similar vehicles. Therefore, understanding the burning and extinguishment characteristics of flames are important for the safe operation of space vehicles. The knowledge gained from such studies is also useful for the safe and efficient use of fuels on Earth. Computer simulations are a cost effective way to obtain data to corroborate limited experimental observations and provide additional details which are difficult to obtain from space based experiments.

Progress During FY 1996:

In addition to uncertainties in the chemical-kinetic input, the assumption of two-dimensionality has been one of the factors hampering quantitative comparisons with experimental data. Therefore, the next step in this research effort is to develop a three dimensional version of the flame code. This is expected to take several months. With the adoption of the time-step or process splitting approach to solve for various physical and chemical processes, the code is very modular. Various processes can be worked on individually and generalized into three dimensions. The first process to be tackled was convection. A three-dimensional version of the basic Flux-Corrected transport algorithm has been implemented. Then, the BIC (barely implicit convection) part of the convective transport was worked on. Finally, the diffusive transport modules were generalized to three dimensions. The entire development was based on using the parallel 2D code as the basis because it would be difficult to run large 3D calculations on conventional vector computers. By the end of last fiscal year (FY95), the entire 3D flame code had been assembled and was being tested against earlier one-dimensional and two-dimensional flame calculations.

The development of the detailed, time-dependent, three- dimensional flame model (FLAME3D) has been completed. The model was developed for MIMD parallel computers and its efficient operation on several machines including the IBM-SP2 and the Intel Paragon have been demonstrated. The developed model is now being used to perform detailed computational studies of the structure and dynamics of premixed flames.

Lean Hydrogen-air mixtures were chosen for the initial study of the three-dimensional structure of cellular flames because earlier two dimensional simulations are available and the chemistry is also well established for these mixtures. The effects of gravity on flames in a 9.5% hydrogen-air mixture was studied by performing and comparing simulations of zero-gravity, upward- and downward-propagating flames. Three- dimensional cellular structures are observed in zero gravity. The cellular flame grows and splits into multiple cells. The growth of the cellular structure is faster in the case of an upward-propagating flame. For the downward-propagating flame, the thermo-diffusive instability mechanism and the gravity induced Rayleigh-Taylor instability mechanism oppose each other, resulting in a nearly planar flame.

Comparing these results to two-dimensional simulations shows that the zero-gravity flames grow more slowly and do not split. This result indicates the need to perform three-dimensional simulations to study these flames. Up to 256 processors of the Intel Paragon and a $192 \times 80 \times 80$ grid was used for the above simulations. These calculations are the first three-dimensional, time-dependent flame calculations with detailed chemistry and transport processes that has been done to our knowledge.

This study was documented in a paper which was presented at the 26th International Symposium on Combustion and has been accepted for publication in the proceedings.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 1/95 EXPIRATION: 12/97

PROJECT IDENTIFICATION: 962-22-05-22

NASA CONTRACT NO.: C-32022-D

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Patnaik, G., Kailasanath, K. and Sinkovits, R., "FLAME3D: a new time-dependent, three-dimensional flame model with detailed chemistry." Paper No. 30, Fall Technical Meeting of the Eastern States Section of the Combustion Institute, Worcester, MA, October 16-18, 1995.

Patnaik, G., Kailasanath, K., and Sinkovits, R.S., "A new time-dependent, three-dimensional, flame model for laminar flames." Presented at the 26th Symposium (International) on Combustion, Naples, Italy, July 1996.

Real Time Quantitative 3-D Imaging of Diffusion Flame Species

PRINCIPAL INVESTIGATOR: Dr. Daniel J. Kane

Southwest Sciences, Inc.

CO-INVESTIGATORS:

Silver, J.

Southwest Sciences, Inc.

Task Objective:

The purpose of this effort is to advance the knowledge of combustion science in reduced gravity environments. The proposed work involves the development of a diagnostic technique to perform simultaneous, spatially- and temporally-resolved measurements of major combustion species and gas phase temperatures. This will be accomplished with a new two-dimensional spectroscopic imaging apparatus.

Task Description:

This approach is predicated on the method of differential absorption spectroscopy. Improved measurement sensitivity will be achieved through the application of high-frequency wavelength modulation spectroscopy. In this fashion, the detection of weak absorbers such as methane and hydroxyl radicals will be pursued. The resulting capability of providing quantitative species data will lead to an improved characterization of microgravity combustion processes as well as providing accurate experimental data to assess and improve the predictive capability of models.

Task Significance:

The development of imaging high-frequency Wavelength Modulation Spectroscopy will enable the ability for the transient, spatially resolved monitoring of weakly absorbing species such as methane and possibly hydroxyl radicals. By coupling the imaging of water vapor with the imaging of methane in diffusion flames it will be possible to localize reaction zones in the flame, leading to a better understanding of the roles of diffusion and buoyancy.

Progress During FY 1996:

The purpose of this project, started in 7/96, is to investigate the fundamental roles of ignition, transport, and chemistry in microgravity diffusion flames by making simultaneous quantitative, spatially-and temporally-resolved measurements of major combustion species and gas phase temperatures. To accomplish this, a new 2-D spectroscopic imaging system will be developed. The instrument will be designed to obtain complete images of temperature and concentration in a single drop. instrument conceptual design has been completed. The original concept of optical demodulation has been abandoned because of DC bleed-through which increases noise. The new design will couple the high frequency data acquisition capabilities of wavelength-modulation spectroscopy and a high speed scanner to obtain images of temperature and concentration. An x-y scanner arrangement will scan the laser over an off-axis paraboloid. Another off-axis paraboloid will focus the laser on to a single high speed detector. This is logistically the same as using the camera which scanned the flame electronically rather than mechanically. At first glance, it might be construed that scanning electronically would be superior; however, mechanical scanning has many advantages. First, the single detector is not limited in well depth, reducing shot noise. Second, the detector is not integrating so that the signal can be electronically demodulated providing a true AC measurement with no DC leakage. This will provide for a more sensitive detection system. Third, faster frame rates may be achieved and the resolution will be adjustable. Fourth, electronic scanning is noisy. Switching noise will leak into the signal path corrupting the signal. As a result of all the advantages of mechanical scanning, optical demodulation was abandoned and a mechanical scanning system is being designed. Currently, several of the electronic boards required for the project have been completed.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/96 EXPIRATION: 6/01

PROJECT IDENTIFICATION: 962-22-05

NASA CONTRACT NO.: NAS3-960

RESPONSIBLE CENTER: LeRC

Soot and Radiation Measurements in Microgravity Turbulent Jet Diffusion Flames

PRINCIPAL INVESTIGATOR: Prof. Jerry C. Ku

Wayne State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objectives of this study are to determine modeling coefficients from measurements of soot morphology and radiation in both normal and reduced-gravity turbulent gas jet diffusion flames, and to further refine models for soot formation and spectrally dependent radiation properties.

Task Description:

In the area of experimental measurements, thermophoretic particle sampling and subsequent transmission electron microscopy analysis are used for soot particle size and analysis of aggregate morphology. Laser light absorption imaging provides for the determination of soot volume fractions. Emission imaging using isolated bandpass filters will be used to measure spectrally dependent soot radiation properties and possibly temperature. Rapid insertion of fine-wire thermocouples will also be used for the determination of temperature.

In the area of modeling, Favre-averaged boundary layer equations with a k-e-g turbulence model and conserved scalar approach with an assumed probability density functions (pdf) are used to predict flow field and gaseous species mole fraction profiles, respectively. The soot formation model has been modified and tested to predict soot volume fraction and number density. The energy equation is included to provide a full coupling between flame structure and radiation analysis. A third-order spherical harmonics approximation and the YIX method have been applied to solve the radiative transfer equation. In the proposed study, soot formation and radiation models will be improved, and methods for efficient spectral integrations and iteration between the solutions for the flame structure and the radiative transfer equation will be sought.

Task Significance:

Microgravity Combustion is not only relevant to fire safety on board a spacecraft, but also provides a unique condition for a better understanding of combustion fundamentals of this common type of combustion.

Progress During FY 1996:

Prior analysis by Ku et al performed under a previous grant consists of the following 4 modeling components:

1. Flow field - k-e(epsilon)-g for turbulence;
2. Combustion - state relationships constructed from CHEMKIN under partial equilibrium (i.e., with heat transfer included);
3. Soot formation and oxidation - a 2-equation model by Moss et al., with soot particle distributions described by scalar transport equations;
4. Radiation heat transfer - by YIX solution, considering soot, CO₂ and H₂O, using Rosseland mean absorption coefficients and neglecting scattering and turbulence-radiation interactions.

These component models perform satisfactorily for laminar flames, in both jet and co-flow configurations. Axial velocity and temperature distributions are accurately predicted. The peak value and the overall shape of soot volume fraction distributions is also be predicted with accuracy. In the present formulation, soot formation model coefficients are allowed to vary for the best fit against experimental data. The resulting values for these coefficients are always physically reasonable, and vary somewhat among different fuels, burners, flow rates and gravity conditions. Further improvement is presently being pursued by the inclusion of more accurate state relationships, such as those based on laminar flamelet models.

The same models performed less satisfactorily for turbulent flames. Resulting predictions for the overall magnitude exhibit close agreement with experimental data, but not the shape of temperature or soot volume fraction distributions. The two most probable causes are attributed to the missing component for turbulence-radiation interactions and the assumed mean absorption coefficients. The turbulence-radiation interactions are viewed as

significant by many researchers, but it remains uncertain about how to account for and model these interactions. Our initial attempt based on the work of Song and Viskanta (AIAA J. Thermophys. Heat Transfer, Vol. 1, 56-62, 1987) has only provided minor improvements. Included in the same formulation is a wide-band model for absorption coefficients similar to that of Song and Viskanta. It appears that the wide-band model does not provide any significant improvement. It is difficult to draw any conclusions at present, due to numerical complexities as well as modeling uncertainties. These modelling issues are presently being pursued.

Based on the modeling results obtained to date, two test matrices are planned:

1. Laminar flames - to provide benchmark data and to further validate the applicability of models. Test matrix - 2 fuels: ethylene and diluted acetylene (maximum optical attenuation less than 20%) or propane (if suitable optical attenuation is observed);

- 1 jet diameter: approx. 3 mm (image only half of the flame);
- 2 fuel velocities: 100 and 150 cm/s;
- 2 gravity conditions: 1-g and 0-g.

2. Turbulent flames - to provide benchmark data and to investigate turbulence-radiation interactions. Test matrix - 1 fuel: ethylene;

- 1 jet diameter: 0.508 mm;
- 3 Reynolds number: 3000, 5000, and 10000;
- 2 gravity conditions: 1-g and 0-g.

Based on this planned matrix, provisions are being made to perform these experiments. Two methods are being pursued for the measurement of temperature; rapid insertion of fine-wire thermocouples, and two-wavelength imaging pyrometry. In the context of the former, calculations verified by the vendor indicate that commercially available, 1 mil thermocouples should provide the necessary temporal response to provide the required gas-phase measurements. The instrument shop is presently being consulted regarding practical considerations for fabricating the thermocouple assemblies. Hardware has been identified and purchased to implement the pyrometry measurements demonstrated by Faeth et al for inclusion in CM-1. Discussions have been conducted with Dr. David Urban, the Project Scientist for CM-1/LSP, regarding calibration procedures and implementation in the 2.2 second drop tower facility.

Provisions are also being made for implementing both 1-g and 0-g velocity measurements via laser doppler velocimetry. Suitable optics and signal processing amenities have been identified, and are being utilized in the laboratory to perform the identified 1-g measurements. The process of integrating this capability into the 2.2 second facility has also been initiated.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 3/95 EXPIRATION: 2/98

PROJECT IDENTIFICATION: 962-22-05-36

NASA CONTRACT NO.: NAS3-126

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Ku, J.C., Toug, L., and Greenberg, P.S. Measurements and modeling of soot formation and radiation in microgravity jet diffusion flames. HTD-vol.335 Proceedings of the ASME Heat Transfer Division, vol. 4, (1996).

Presentations

Ku, J.C., Toug, L., and Greenberg, P.S. "Detailed modeling analysis for soot formation and radiation in microgravity gas jet diffusion flames." Third International Microgravity Combustion Workshop, Cleveland, OH, April 11-13, 1995.

Studies of Flame Structure in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Chung K. Law

Princeton University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objectives of this work are to understand and quantify the structure, stabilization mechanisms, soot formation in, and extinction of one-dimensional premixed and nonpremixed laminar flames.

Task Description:

This program comprises two main elements:

1. A numerical simulation of one-dimensional laminar flames is to be developed that, in addition to including the usual fluid mechanical and heat transfer mechanisms, will include detailed chemical kinetic mechanisms for comparison with the unique experimental results.
2. A drop-tower test apparatus is to be used to observe premixed laminar flames stabilized about cylindrical and spherical porous burners to distinguish heat loss and flow divergence influences on flame stabilization and flamefront stability.

Task Significance:

The one-dimensional adiabatic laminar unstretched premixed flame is a fundamental precept of combustion science, but cannot be stabilized in normal gravity because of the straining or asymmetrical influences of gravitationally induced buoyant convection. In microgravity experiments, this program demonstrates this combustion paradigm and provides a capability for probing the structure, chemistry, soot dynamics, and flame propagation speed of these fundamental flames.

Progress During FY 1996:

- 1) Spreading of Unsteady Cylindrical Diffusion Flames: It is well known that while a steady solution exists for spherical diffusion flames, cylindrical diffusion flames are intrinsically unsteady. In the presence of gravity, distortion of the flame shape could lead to a stabilized steady-state, complex three-dimensional flame configuration. However, in the absence of gravity, upon ignition a cylindrical flame is expected to continuously spread out to the ambient. In this study we have theoretically analyzed the spreading rate, and found that the extent of unsteadiness is critically dependent upon the ambient oxidizer concentration. Specifically, for high oxidizer concentrations, the spreading rate of the flame lags that of diffusion such that the flame behaves quasi-steadily, while the opposite holds for small oxidizer concentrations such that the flame spreads out unsteadily. These characteristics of flame dynamics will be experimentally investigated in the microgravity environment.
- 2) Response of Spherical Premixed Flames under Rotation: The influence of burner rotation on an otherwise spherical premixed flame was analytically studied. The results show that with rotation, the flame deforms into a pancake shape that may be flattened either at the poles or the equator, depending upon the combined effects of Lewis number, flame stretch, and ambient temperature. Implications on the extinction locations over the flame surface are also indicated.
- 3) Extended Limits of Flammability: Recent microgravity results on near-limit counterflow flames showed that, for lean methane/air flames whose Lewis number is less than unity, the combined effects of mixture nonequidiffusion and positive stretch elevated the combustion intensity such that steady burning persists beyond the fundamental flammability limit defined for the one-dimensional flame. Furthermore, the flame response to stretch rate variations exhibits a dual extinction turning point behavior in that flame extinction occurs not only for sufficiently large stretch rates and minimal radiative heat loss, but also for sufficiently small stretch rates and relatively substantial heat loss. Such an enhancement in burning however was not observed for lean propane/air flames whose Lewis number is larger than unity. In the present study we have computationally simulated the

microgravity experiment and reproduced the experimental observations. Enhanced insights into the extinction mechanisms of such limit flames were also obtained.

4) **Dual Luminous Zone Structure of Diffusion Flames:** Micro-buoyancy experiments on diffusion flames of methane/hydrogen versus air reveal a flame structure consisting of two luminous zones. Subsequent studies on counterflow flames show a similar structure, although less prominent. The structure of such a flame is currently being studied computationally.

5) **Microgravity Experiments on Spherical Diffusion Flames:** Microgravity experiments conducted on burner-generated spherical diffusion flames showed that the flame continuously increases in size during the drop. Preliminary estimates reveal that although a steady-state configuration should exist, the unsteadiness due to fuel vapor accumulation could lead to the observed unsteadiness during the finite time available for the 2.2 second drop. Computational simulation is currently being conducted to check on this hypothesis.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	2	PhD Degrees:	2

TASK INITIATION: 5/90 EXPIRATION: 5/98

PROJECT IDENTIFICATION: 962-22-05-37

NASA CONTRACT No.: NAG3-171

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Qian, J., and Law, C.K. On the spreading of unsteady cylindrical diffusion flames. Combustion and Flame, (accepted 1996).

Qian, J., Bechtold, J.K. and Law, C.K., On the response of spherical premixed flames under rotation. Combustion and Flame, (accepted 1996).

Presentations

Sung, C.J., and Law, C.K. "Extinction mechanisms of near-limit premixed flames and extended limits of flammability." 26th International Combustion Symposium, Naples Italy, 1996.

Chemical Inhibitor Effects on Diffusion Flames in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Gregory T. Linteris

National Institute of Standards and Technology

CO-INVESTIGATORS:

Hochgreb, S.

Massachusetts Institute of Technology (MIT)

Task Objective:

The objectives of the proposed research are as follows:

1. To determine the effects of flame inhibitors on the physical characteristics (height, shape, color, and luminosity) and stability limits (ignition, extinction, lift-off and blow-off) of gaseous diffusion flames in the presence of halogenated fire suppressants in microgravity.
2. To develop quantitative analytical models for the observed behavior, including chemical kinetic effects, in order to understand the mechanisms of inhibition of halogenated compounds in gaseous diffusion flames.

Task Description:

The experiments will consist of normal and microgravity studies of laminar jet and co-flow diffusion flames inhibited by halogenated suppressant addition to the air or fuel stream. In microgravity, visual and temperature diagnostics will be utilized to detect flame shape, dynamics and stability limits. Normal gravity experiments will make use of additional chromatographic and spectroscopic diagnostics in addition to visual and temperature measurements.

Analytical and computational work will be performed using existing general 2-D codes with chemical kinetic models for comparison with the observed results. The calculations should serve for comparison with observations, explanation of observations and selection of additional experimental conditions of interest.

Task Significance:

Fire suppression in space is one of the main reasons to investigate combustion phenomena in microgravity. Since halogenated compounds will remain as the fire suppressant of choice in many space missions, there is clearly a need for experimental evidence on the effectiveness of these compounds under zero buoyancy conditions.

The final product of the experimental and analytical work is a comprehensive and quantitative understanding of the physical and chemical phenomena involved in the suppression of diffusion flames through the addition of chemical halogenated inhibitors. This understanding is expected to be very useful both from a fundamental viewpoint as well as for the practical utilization of chemical fire suppressants in space.

Progress During FY 1996:

Status

1. Analyzed the experimental results of hypotheses that could lead to a better interpretation of our current database on the behavior of laminar jet diffusion flames in microgravity and normal gravity experiments with and without chemical inhibitor (CF₃H and CF₃Br) addition, and documenting the findings. Topics covered include multiple-zone structure of CF₃Br inhibited flames, open-tipped behavior, soot reduction of CF₃H inhibited flames, and the effects of oxygen concentration, increased flow rate, and pressure. A publication is currently in preparation.
2. Developing diagnostics that may be added to the experimental setup to determine the temperature field. A prototype imaging interferometer (similar to that used by Liu and Ronney, 1995) was built to investigate the behavior of diffusion flames, and work is under way to perform quantitative deconvolution of the fringes into temperature measurements. Potential expected difficulties include making more accurate estimations of the indices of refraction and deflection of the beam by the flame.

3. Testing available CFD codes for aiding in the interpretation of the results. A CFD code was used along with a one step reaction mechanism to investigate the effect of flame dilution by nitrogen (one of the test cases) compared to a baseline case. Convergence was hampered by the entrained flow nature of the laminar jet flow. A compromise was reached by starting the calculation with a co-flow condition with a 1:100 ratio for the air flow relative to the jet flow. Although the code has limited capabilities for chemical kinetics, insight can be gained from the calculated temperature are varied. We have just been granted 200 CRUs of super-computing time at NCCS, and we will be looking for alternative calculation schemes that would allow introduction of additional chemistry, possibly in cooperation with other investigators.

APRIL - JUNE

During this quarter, modifications to the ground-based apparatus at MIT were completed. The system is now capable of maintaining a flame continuously at low pressure. A coflow system with flow straighteners was added to provide the flame with fresh oxidizer. The oxidizer mixture is supplied through flow meters to allow addition of inhibitor to the oxidizer stream. A vacuum regulator was added to keep the pressure constant while removing the products. Water scrubbers were also added to the evacuation system to protect the vacuum pump from the halogen halides produced from the inhibitors. Two dimensional probing capabilities were also added to the apparatus, for use with thermocouples or gas sampling probes. Axial adjustment is accomplished by moving the burner/coflow assembly vertically. Radial adjustment is provided by a sealed micrometer inserted through one of the side window ports.

Also this quarter, further preparation has been made for the use of a interferometric temperature diagnostic. A laser and associated optics have been ordered, and initial packaging schemes for use in a drop rig have been devised. The analysis method for the fringe patterns is almost completed. Subroutines for data extraction from the images and for FFTs are already complete, and the deconvolution of the temperature field is being implemented. Plans for the next set of microgravity experiments in September are to utilize this diagnostic to investigate the temperatures of the inhibited flames during the experiment.

Computations have been started at NIST to complement the ongoing laminar jet diffusion flame experiments. In direct numerical simulations, time dependent simulations of an axisymmetric laminar jet diffusion flame without coflow are in progress for flames in both normal and microgravity. The code uses a simple mixture fraction based model for combustion. In previous work, both the instantaneous and time-averaged behavior of pool fires and isothermal helium plumes have been successfully simulated. Although computer time on a NASA super-computer was obtained, the calculations are in progress on NIST machines because of faster turn-around times. Modifications continue to obtain a converged solution.

4th Quarter

Over the past quarter, the interferometric temperature measurement diagnostic being developed at MIT for the 2.2 Second Drop Tower was completed and implemented. The objective of the additional instrumentation is to provide temperature field measurements for both ground and drop-tower experiments.

The diagnostic consists of an optical setup mounted on a plate designed to be installed in one of NASA's PIG-rigs. The diagnostic operates by passing an expanded, slightly-diverging beam from a Helium-Neon laser through the flame and immediate vicinity. Two samples of the beam are then reflected from the faces of an uncoated piece of glass. These two reflections interfere on a screen. The interference pattern is recorded to video using a black-and-white CCD camera. Changes in the fringe spacing therefore depict changes in the gas density in the beam path, which can be related to changes in gas temperature. To get absolute temperatures, a thermocouple is used to record the temperature at the edge of the beam. A color CCD camera is also included to record the visible emissions from the flame.

During the first week of September, this diagnostic was brought to NASA LeRC and assembled onto the 2.2 Second Drop rig PIG-1. Only a couple of preliminary drops were made before the air bag failed. The next two weeks were then used to make slight modifications to the diagnostic. The preliminary drops showed the temperature gradients in microgravity were much more shallow and existed further from the flame than in normal gravity. Therefore, a smaller nozzle was selected, the optics were adjusted for higher sensitivity, and a thermocouple was added (rather than assuming ambient temperature). During the week of September 23, the diagnostic was reassembled and a set of data points covering the base of the previous set (except for the nozzle diameter) was tested.

An appropriate software has been developed for the analysis of the interferometric images. The program can currently perform FFT's and shift the data to remove the carrier frequency. Additional subroutines are being developed to deconvolute the data and perform the Abel transform to extract the radial temperature profiles.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 0

PhD Students: 1

TASK INITIATION: 6/94 EXPIRATION: 6/98

PROJECT IDENTIFICATION: 962-22-05-54

NASA CONTRACT No.: C-32016-C

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

VanDerWege, B.A., Bush, M.T., Hochgreb, S., and Linteris, G.T., "Effect of CF₃H and CF₃Br on laminar diffusion flames in normal and microgravity." Eastern States Section Meeting/The Combustion Institute, Worcester, MA, October 1995.

Computational and Experimental Study of Laminar Diffusion Flames in a Microgravity Environment

PRINCIPAL INVESTIGATOR: Prof. Marshall B. Long

Yale University

CO-INVESTIGATORS:

Smooke, M.D.

Yale University

Task Objective:

The objective of this work is to use a combined computational and experimental approach in microgravity to study the formation of combustion-generated pollutants, such as soot, NO_x, and unburned hydrocarbons, in laminar diffusion flames.

Task Description:

Experimental and computational procedures will be applied to laminar diffusion flames in both normal and microgravity conditions. Microgravity conditions increase the length scales such that increased resolution of both major and minor species will be possible, thus reducing the demands placed on both the computational and diagnostic tools. Results of a detailed transport/finite rate chemistry model will be compared with nonintrusive optical diagnostic measurements of the structure and extinction of both sooting and nonsooting hydrocarbon-air flames.

Task Significance:

A combined computational and experimental approach in a microgravity environment will study the formation of combustion-generated pollutants, such as soot, NO_x, and unburned hydrocarbons, in laminar diffusion flames. The results of combined normal gravity and microgravity studies will contribute to an understanding of pollutant formation in flames and its relation to the design of the next generation of combustors that will be able to burn cleanly and efficiently.

Progress During FY 1996:

This investigation began July 31, 1996. The PI visited LeRC soon after and met with the 2.2 Second Drop Tower and DC-9 facility managers. Discussion on facility capabilities and constraints was conducted to assist the PI on choosing the facility for his microgravity studies. Plans were made for the PI and Co-I to run calculations to determine the estimated sensitivity of their flames to the various g-levels.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/96 EXPIRATION: 7/00

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NAG3-193

RESPONSIBLE CENTER: LeRC

Dynamics of Liquid Propellant Combustion at Reduced Gravity

PRINCIPAL INVESTIGATOR: Dr. Stephen B. Margolis

Sandia National Laboratories

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The project is an analytical study, calculating the physical characteristics and the time-related dynamics (pulsations, for example) of a liquid-propellant pyrolysis and combustion system. The modeling incorporates reduced gravity as a parameter, since it has been found that gravity is a significant influence on the dynamic behavior of the liquid-gas interface and consequently the overall combustion process.

Task Description:

The analysis adapts an existing model of the dynamics of fluid and thermal behavior in liquid-propellant systems, as developed by the Principal Investigator in prior studies. In this model, combustion is deemed to take place in the neighborhood of the liquid/gas interface. This is true for the combination of hydroxylammonium nitrate-based propellants modeled in the previous studies, but it is also an adequate representation for more generalized cases of gas-phase and spray combustion.

The principal focus of the modeling is the prediction of reactive/diffusive instabilities as well as hydrodynamic instabilities in the combustion field. The innovation in the current analyses is in the formal scaling of gravitational acceleration explicitly in the calculations. This requires a complete reformulation of the problem, offering the promise of novel information representative of the performance of reaction systems at varying gravity levels approaching zero.

The calculations are to cover a range of input parameters including liquid-gas density and viscosity variations. The model output will be in the form of maps of the stability boundaries, with complete descriptions of the reactive fields and their properties, for generalized applications.

Task Significance:

The application of the models and analyses of the study has direct significance to existing and proposed rocket-propulsion systems. Specific and generalized information will be useful in designs and operational modifications for improved and stable combustion performance in liquid-propellant engines, particularly those operated in low-gravity fields, such as in upper stage propulsion and orbital maneuvering.

Progress During FY 1996:

The project initiated in the final months of the fiscal year. The Principal Investigator has established the requirements and boundaries of the analyses and has defined the initial steps necessary to modify and extend the prior model of liquid-propellant combustion to incorporate variable gravity as a parameter.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-22-05-73

NASA CONTRACT NO.: C-32031-E

RESPONSIBLE CENTER: LeRC

Structure and Dynamics of Diffusion Flames in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Moshe Matalon

Northwestern University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objectives of the work are to gain insight into diffusion flames by studying simple combustion systems. The emphasis of the work will be to understand the structure and dynamics of stationary spherical flames, and the coupled processes occurring in the liquid and gas phases associated with the burning of liquid fuels.

For gaseous flames, the Principal Investigator will investigate the processes that lead to extinction of these flames either by the process of blowoff or by radiative losses. He will also examine the nature of the interactions between two diffusion flames, the mechanisms leading to the generation of flame front instabilities, the formation of cellular flames and the effect of residual gravitational acceleration on microgravity diffusion flames.

For liquid fuel burning, the Principal Investigator will examine the possible generation of instabilities that are intrinsic to the vaporization process and identify the importance of thermocapillary motion on the overall burning process.

Task Description:

The program is entirely theoretical in nature. The Principal Investigator will work closely with related experimental investigations in the microgravity combustion science program to identify problems of specific interest.

The porous sphere will be the model problem for gaseous diffusion flames. A standard formulation of the conservation equations in spherical coordinates forms the base case. The model will then be extended to incorporate finite rate kinetics through activation energy asymptotics, enabling details of the flame structure to be elicited. The model can then be extended to include a standard form of a radiative loss to determine the extinction limits, blowoff and radiative, of the combustion system. Finally, the model will be extended to determine the effects of interaction by modeling two spherical diffusion flames in close proximity to each other employing bi-spherical coordinates in the approach outlined above.

As a next step the core model will be extended to incorporate stability theory and determine the conditions for the onset of flame-front instabilities similar to those that have been observed experimentally. Similarly, the effect of a low-magnitude, time-varying body force (g -jitter) on the flame will be examined, by casting the disturbance as a sinusoidal term in the governing equations.

The ideas developed above will then be extended to liquid fuels. The major change to the model will be the incorporation of the liquid phase, the conservation equations for the liquid phase, and the coupling of the gas and liquid phases. A major addition will be the incorporation of thermocapillary motion in the liquid phase equations.

Task Significance:

The proposed research will lead to a greater understanding of diffusion flames in general. By working closely with experimental studies in the microgravity science program, the investigator will be able to give a theoretical foundation to many experimental observations of diffusion flames in microgravity.

Progress During FY 1996:

Near Limit Oscillations of Diffusion Flames

Motivated by the near-limit oscillations of candle flames observed in microgravity experiments, we have conducted a study that examines the dynamics of diffusion flames under conditions similar to the ones found in the experiments. More specifically, we have examined the behavior of the diffusion flame when the ambient oxidant concentration is

low. A diffusion flame may be characterized by the response of the burning rate to a properly defined Damkohler number, representing the ratio of diffusion time to chemical reaction time. An alternative characterization is the dependence of the burning rate on the ambient oxidant concentration, for a fixed Damkohler number. In either case typical response curves are either S-shaped or monotonic curves. While the S curve exhibits ignition and extinction phenomena, the monotonic curve indicates that there is a gradual transition from intense burning to a nearly frozen state and vice-versa. Stability considerations indicate that spontaneous oscillations develop when the Lewis number is sufficiently large and/or heat losses are excessive. This suggests that the ignition/extinction conditions, normally associated with the turning points of the S curve, must be modified and related to the points of exchange of stability. For a monotonic response curve the oscillations lead to extinction that is not predicted otherwise. The near-limit oscillations predicted here are qualitatively similar to the ones observed in the microgravity candle flame experiment, and the frequencies of oscillations predicted are of the same order of magnitude.

Pool Fires and Burning Liquid Films

A numerical study of the stability of a one-dimensional diffusion flame above a liquid pool has been carried out. The analysis identifies a diffusional-thermal instability obtained when the Lewis number of the fuel is sufficiently large.

The stability of a thin film that burns at a diffusion flame has been analyzed. The problem is inherently unsteady and exhibits a strong coupling between the liquid and gas phases. Using a long wavelength approximation, an evolution equation that describes the instantaneous shape and position of the free surface has been derived. Results pertaining to the stability of the interface have been discussed. The flame tends, in general, to stabilize the liquid film. An instability may result along the film interface when the flame is located far enough from the surface and the mean liquid temperature is relatively large.

Flame Spread over Solid Surface

A well known model for flame spread over a solid fuel surface is due to de-Ris. Assuming an infinite Damkohler number, which implies a thin diffusion flame sheet along which both fuel and oxidant are completely consumed, the formulation lends itself to a Weiner-Hopf problem. Our objective is to determine the spread rate when fuel and oxidant are permitted to leak through the flame sheet. Preliminary results indicate that there will be a reduction in spread rate. Whether this could lead to flame extinction is a question that remains to be addressed.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 6/94 EXPIRATION: 5/98

PROJECT IDENTIFICATION: 962-22-05-47

NASA CONTRACT No.: NAG3-160

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Cheatham, S. and Matalon, M., Near-limit oscillations of spherical diffusion flames. AIAA Journal, (1996).

Fisher, I., Buckmaster, J., Lozinski, D. and Matalon, M., Vapor diffusion flames, their stability, and annular pool fires. Mathematical Modeling in Combustion Science, Springer Verlag, pp. 249-257 (1995).

Matalon, M., Flame propagation in closed vessels. Mathematical Modeling in Combustion Science, Springer Verlag, pp. 163-175 (1995).

Presentations

Cheatham, S. and Matalon, M., "Near-Limit Oscillations of Spherical Diffusion Flames ." AIAA Paper 96-0260, 34th Aerospace Sciences Meeting and Exhibit, 1996.

Cheatham, S. and Matalon, M., "Heat Loss and lewis number effects on the onset of oscillations in diffusion flames ." Twenty-Sixth Symposium (International) on Combustion, 1996.

Matalon, M. "Modelling combustion phenomena." Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland, 1995.

Matalon, M., "An evolution equation describing the propagation of premixed flames in closed tubes." 48th Annual Meeting of the Division of Fluid Dynamics, American Physical Society, Irvine, CA, 1995.

Matalon, M., "Near limit oscillations of spherical diffusion flames." 34th Aerospace Sciences Meeting and Exhibit, American Institute of Aeronautics and Astronautics, Reno, Nevada, 1996.

Matalon, M., "Flame propagation in closed tubes." Sixth International Conference on Numerical Combustion, New Orleans, Louisiana, 1996.

Filtration Combustion for Microgravity Applications: (1) Smoldering, (2) Combustion Synthesis of Advanced Materials

PRINCIPAL INVESTIGATOR: Prof. Bernard J. Matkowsky

Northwestern University

CO-INVESTIGATORS:

Bayliss, A.

Northwestern University

Volpert, V.A.

Northwestern University

Task Objective:

The objective is to investigate combustion in porous media with applications to (1) smoldering and (2) combustion synthesis of advanced materials, also referred to as self-propagating high-temperature synthesis (SHS).

Task Description:

The task involves (1) Proposing/developing theoretical models describing the fundamental mechanisms for the phenomena under consideration, (2) performing complementary analytical and numerical work on the proposed models and mechanisms, and (3) comparing the results of these analyses to experiments.

Task Significance:

Both smoldering and combustion synthesis of advanced materials (SHS) contribute to fundamental science, and also represent important applications for microgravity combustion science; in smoldering to fire safety in both normal and microgravity, and in SHS to the determination of optimal synthesis conditions in both normal and microgravity environments. Combustion synthesis appears to compete favorably with conventional technology, by achieving shorter synthesis times, and at lower cost, by employing the internal energy of the combustion reactions rather than the costly external energy of a furnace, employed in conventional technology.

Progress During FY 1996:

A paper entitled "Gravity Induced Separation in 'Liquid Flames'," by K.G. Shkadinsky, G.V. Shkadinskaya and B.J. Matkowsky is accepted to Combustion Science and Technology for publication. The Abstract of the paper reads: "We study the structure of a combustion wave propagating through a heterogeneous powder mixture which initially forms a hard matrix. The matrix is destroyed by the propagating combustion wave, due, e.g., to melting of some of the components of the mixture. Thus, a liquid bath is formed, in which processes such as heat and mass transfer as well as chemical reactions determine the structure of the combustion wave, its propagation velocity and the composition of the reaction product. The liquid bath is a suspension containing particles, either liquid or solid, which may either be reactive or inert. Under the influence of gravitational forces there is the possibility of relative motion of the individual components of the mixture, especially when the sample is subject to the action of an external force field. This may result in separation of the components under the influence of an external force field, such as gravity, if the densities of the components differ from one another. Separation is opposed by a friction force. To gain an understanding of the phenomena associated with relative motion and separation during the propagation of the combustion wave, topics which heretofore have not been considered, we formulate and analyze a relatively simple mathematical model of "liquid flame" combustion in a gravitational force field. We determine the structure of uniformly propagating combustion waves and describe the possibility of multiplicity of such solutions. We also consider nonstationary waves and show that "shock" type solutions, with jumps in the composition of the sample, are possible."

A paper entitled "Downward Buoyant Filtration Combustion," by A.P. Aldushin, B.J. Matkowsky and D.A. Schult is accepted for publication in Combustion and Flame. The Abstract of the paper reads: "We consider heterogeneous combustion in a porous medium subject to gravity induced buoyant forces. A vertical sample, open to flow at the top and bottom, is ignited at the top. Buoyancy causes the hot gases to leave the sample through the top, thus drawing in fresh cool gas, containing both oxidizer and inert gases, through the bottom. The incoming gas supplies the reaction with oxidizer. In contrast to forced filtration, in which the flux of gas into the sample is prescribed, here the incoming flux is determined by the combustion process itself. This configuration describes smoldering, self-propagating high-temperature synthesis (SHS) of advanced materials, and a host of other applications. Combustion waves are described for both adiabatic and non-adiabatic conditions in which heat is lost to the external

environment through the sides of the sample. The heat loss causes the temperature in the product to decay from the combustion temperature to the temperature of the external environment in a region termed the cooling region. Two non-adiabatic cases are considered, distinguished by whether or not the sample is sufficiently long and the heat losses sufficiently large that the cooling region behind the reaction site is completely contained within the sample. When it is totally contained in the sample we describe traveling wave solutions whose shape does not change in time, provided there is no net production of gas in the reaction. When it is not completely contained within the sample, we describe quasi-steady combustion waves which change slowly in time due to the increasing buoyant flux as the combustion wave penetrates further and further into the sample. Solutions are categorized as gas deficient when the oxidizer is completely consumed, solid deficient when the solid fuel is completely consumed, or stoichiometric when both oxidizer and solid fuel are completely consumed. Extinction is found to occur for solid deficient and stoichiometric solutions when the buoyant flux is sufficiently large. We show that in order to ignite a self-sustained combustion wave, sufficient heat must be supplied so that in addition to providing a sufficiently high temperature to form a preheat layer, there is sufficient buoyant flux of oxidizer to allow the combustion wave to become self-sustained. In particular, combustion will not occur in microgravity environments unless there are other mechanisms of oxidizer transport. Some samples will not support a combustion wave because the flux required for ignition is larger than the critical level for extinction. Under non-adiabatic conditions, another extinction mechanism exists in which heat loss lowers the temperature below a critical level. The results of our analysis compare favorably with experimental observations of downward buoyant combustion in the region away from the ends of the sample."

A paper entitled "Upward Buoyant Filtration Combustion," by A. Aldushin, B.J. Matkowsky and D.S. Schult has been submitted to the J. Engineering Mathematics for publication.

A paper entitled "Gravitational Effects on the SHS Production of High Porosity Materials," by K.G. Shkadinsky, G.V. Shkadinskaya and B.J. Matkowsky is accepted to Combustion Science and Technology for publication. The Abstract of the paper reads: "We introduce a model of combustion of porous samples in a gravitational field, in which the high temperature products can deform, to describe the synthesis of high porosity materials and its dependence on parameters of the problem. In addition to the main synthesis reaction we allow for the possibility of a gasification reaction of a special additive. We derive an equation for the elongation of the sample due to an increase in its porosity, which is caused by the additional gas produced in the main reaction or in the additive reaction or both. We also carry out numerical simulations of the model and compare to existing experimental results. We describe ignition, propagation, extinction and stability of propagating combustion waves and their dependence on various factors such as heat loss, gravity, rheological parameters and amount of additive. In particular, we show the possibility of synthesizing uniform high porosity materials in a microgravity environment."

A paper entitled "Enhancement of Gasless Combustion Synthesis by Counterflow Gas Filtration," by A.P. Aldushin, B.J. Matkowsky, and V.A. Volpert is published in Combustion Science and Technology. The Abstract of the paper reads: "We study the propagation of combustion waves through porous samples in which two reactions occur. The first is a gasless solid-solid reaction between two solid species in the porous solid matrix which react to synthesize a solid product. The second is a solid-gas reaction in which gas, delivered to the reaction site through the pores of the sample, reacts with one of the solid species to form gaseous products. We consider the case of counter-flow filtration, in which the direction of gas flow is opposite to the direction of propagation of the reaction wave. Our purpose in considering such systems is that the solid-solid reaction is sometimes only weakly exothermic or even endothermic, so that propagation, and therefore synthesis, in the absence of enhancement of the reaction rate would not be possible. Enhancement is achieved by arranging for counterflow gas filtration, which leads to the solid-gas reaction. Heat released in the solid-gas reaction raises the temperature in the combustion wave, thus increasing the solid-solid reaction rate. Using the large activation energy approximation, which describes narrow reaction zones, we determine the structure and characteristics of the combustion wave."

A paper entitled "Stability of Uniformly Propagating SHS Waves in Porous Solids with Melting and Flow of Reactants," by C.S. Raymond and V.A. Volpert is accepted to Chemical Engineering Science. The Abstract of the paper reads: "We formulate a two dimensional model describing the combustion of porous condensed phase materials in which a reactant melts and spreads through the void space of a porous solid. The melt may completely fill the pores, or some gas may remain in the pores. In each case, the volume fraction of melt is prescribed. In the limit of large activation energy, we analytically find a one dimensional basic state consisting of a uniformly

propagating combustion wave with a planar reaction front and a planar melting front. We find that the uniformly propagating solution with planar fronts is unstable to traveling waves transverse to the propagation direction of the basic state above some critical Zeldovich number. The critical wave number associated with the critical Zeldovich number is generally unique and nonzero. However, the critical wave number can be zero for certain parameter values. For other special parameter values, the neutral stability curve may have two minima, so that two wave numbers lose stability at the same Zeldovich number."

A paper entitled "Stabilization of Gasless Combustion Waves by High Melting Temperature Additives," by C.S. Raymond and V.A. Volpert is accepted to the International Journal of SHS for publication. The Abstract of the paper reads: "Self propagating high temperature synthesis (SHS) is a technique for producing a wide variety of useful inorganic materials using combustion waves. There are several modes in which a combustion wave can move through the reactants, but practitioners of SHS usually desire the uniformly propagating combustion wave, in which a planar reaction front moves through the mixture of reactants with a uniform speed, since this mode of combustion leads to the most uniform product and the greatest conversion of reactants to products. Previous theoretical work has demonstrated that the presence of low melting temperature components in mixtures to be processed by SHS may lead to destabilization of the uniformly propagating combustion wave. We perform a linear stability analysis and show that this destabilization may be countered by the addition of an inert with a high melting temperature."

A paper entitled "Stability of 'Liquid Flame' Combustion Waves," by K.G. Shkadinsky, G.V. Shkadinskaya and V.A. Volpert is submitted to Chemical Engineering Science. The Abstract of the paper reads: "We study combustion waves propagating through a heterogeneous powder mixture which initially forms a hard porous matrix. The matrix is destroyed by the propagating combustion wave, due, e.g., to melting of some of the components of the mixture. Thus, a liquid bath is formed which contains a suspension of particles. The burning of the sample occurs in a gravitational field. If the gravitational field is sufficiently strong, and the densities of the species sufficiently different, then there is relative motion of the components which affects the composition of the species in the combustion wave, its structure, and therefore, the stability of the propagating wave. Depending on the direction of propagation of the wave and the relation between the densities of the species, two different processes can occur. One is the separation process which occurs either when the combustion wave propagates downward (i.e., in the direction of gravity) and the initial reactant is heavier than the product, or when the combustion wave propagates upward and the initial reactant is lighter than the product. The other is the mixing process which occurs in the opposite situations. We find the characteristics of the uniformly propagating combustion waves in such systems and show that generically the mixing process stabilizes, while the separation process destabilizes the propagation of the combustion wave."

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	1
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 5/94 **EXPIRATION:** 5/98

PROJECT IDENTIFICATION: 962-22-05-55

NASA CONTRACT NO.: NAG3-160

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:
Journals

Aldushin, A.P., Matkowsky, B.J., and Schult, D.A., Downward buoyant filtration combustion. Combustion and Flame, (accepted 1996).

Aldushin, A.P., Matkowsky, B.J., and Volpert, V.A., Enhancement of gasless combustion synthesis by counterflow gas filtration. Combustion Science and Technology, vol. 103, pp. 1-20 (October 1995).

Raymond, C.S., and Volpert, V.A., Stability of uniformly propagating SHS waves in porous solids with melting and flow of reactants. Chemical Engineering Science, (accepted 1996).

Raymond, C.S., and Volpert, V.A., Stabilization of gasless combustion waves by high melting temperature additives. International Journal of SHS, (accepted 1996).

Schult, D.A., Matkowsky, B.J., Volpert, V.A., and Fernandez-Pello, A.C., Propagation and extinction of forced opposed flow smolder waves. Combustion and Flame, vol. 101, pp. 471-490 (October 1995).

Schult, D.A., Matkowsky, B.J., Volpert, V.A., and Fernandez-Pello, A.C., Forced forward smolder combustion. Combustion and Flame, vol. 104, pp. 1-26 (1996).

Shkadinsky, K.G., Shkadinskaya, G.V., and Matkowsky, B.J., Gravity induced separation in liquid flames. Combustion Science and Technology, (accepted 1996).

Shkadinsky, K.G., Shkadinskaya, G.V., and Matkowsky, B.J., Gravitational effects on SHS production of high porosity materials. Combustion Science & Technology, (accepted 1996).

Shkadinsky, K.G., Shkadinskaya, G.V., and Volpert, V.A., Stability of liquid flame combustion waves. Chemical Engineering Science, (accepted 1996).

Combustion of PTFE: The Effect of Gravity on Ultrafine Particle Generation

PRINCIPAL INVESTIGATOR: Prof. J. T. McKinnon

Colorado School of Mines

CO-INVESTIGATORS:

Todd, P.W.
Oberdorster, G.University of Colorado
University of Rochester

Task Objective:

The project is an experimental and analytical study of the fundamental chemical and physical mechanisms and the influence of gravity on the ultrafine particles and gases generated by the thermal breakdown of polytetrafluoroethylene (PTFE) wire insulations. PTFE is a widely used spacecraft material that resists ignition and fire spread, but it can degrade when stressed by thermal and electrical overloads to release ultra-fine (10 to 100 nm) particles as aerosols or smoke.

Task Description:

The experimental study is performed in four phases.

1. Normal-gravity tests, conducted at the Colorado School of Mines, investigate PTFE powder, or a reference perfluorinated alkane, in a flow-tube reactor under three atmospheres—wet air, dry air, and nitrogen. The reaction-temperature range is from 380 to 700 C. The gas products are collected and analyzed using gas chromatography and mass spectrometry. The concentration of ultrafine particles in the effluent gas stream (smoke) is measured using optical absorption. The particles are also collected on filters and analyzed chemically and physically by Fourier transform infrared spectroscopy (FTIR) and electron microscopy.
2. Normal-gravity tests, conducted at the Colorado School of Mines, investigate the smoke emitted from a PTFE-insulated copper wire thermally overloaded in a closed chamber under wet air, dry air, and nitrogen. In these tests, smoke density is measured by light scattering, and representative samples of the particles are collected by thermophoresis.
3. Microgravity tests, conducted in the Colorado School of Mines 1.2-sec air drop tower, investigate the effect of gravity on the degradation reaction and product evolution. The test apparatus is a modification of the closed chamber used in the Phase 1 study, supported and mounted on a frame for drop-tower recovery.
4. Microgravity tests, conducted in the NASA Lewis Research Center drop-tower and airplane facilities, extend the investigations of the preceding task to longer times of low-gravity exposure and a greater variety of test parameters. These test requirements will be developed from the results of the preceding studies.

The accompanying analytical study develops a comprehensive model to predict ultrafine-particle production, given inputs of heating rate, polymer quantity, degree of forced convection, and other factors. This analysis is based on elementary reaction rates from established databases, the Principal Investigator's previous studies on soot formation, and the interpretations of the results of the experimental tests.

Task Significance:

The study will examine the phenomenon of ultrafine-particle generation from the thermal degradation of fluorocarbon polymers widely used in aircraft and spacecraft wire insulation. Testing at low gravity offers insights into the chemical and physical influences on the polymer degradation processes and the generation of potentially toxic aerosols. Microgravity also provides the environment to model spacecraft hazard scenarios for a greater understanding of the ultrafine-particle phenomena, offering the promise of a reduction of health and fire threats in space.

Progress During FY 1996:

The experimental studies conducted in the current year concentrated on the normal-gravity and microgravity behavior of heated wires with polytetrafluoroethylene (PTFE) insulations in ordinary air environments, namely, Phases 2 and 3 of the Task Description.

The test articles are 20 AWG silver-plated copper wires insulated with PTFE, mounted within a transparent containment box. The wires, supported in an inverted U-shape, are heated ohmically by overload currents. Diagnostics include camera imaging of the effluent "smoke" as illuminated by a laser light sheet, collection of effluent particles on a thermophoretic probe, and physical analysis of the collected particles and aggregates. Earlier tests in a tube furnace determined the compositions of gases in the effluents.

The apparatus was mounted in a compact, well supported frame, enabling recovery from the deceleration shocks of drop-tower testing. The frame is also compatible with the NASA Lewis drop-tower and airplane requirements, for future testing in these venues.

Qualitative results from the imaging show that, under normal gravity, the aerosols generated by the degrading PTFE insulations form a long upward plume above the wire that remains laminar during the test times of almost three seconds (limited by failure of the copper wire). Under microgravity, the particles form a near-symmetric sphere around the overheated wire. The microgravity test times, of course, are limited to a little more than one second, and they do not extend to wire failure.

Particles were collected from 21 microgravity experiments to date, each associated with a normal-gravity test at corresponding conditions. Under normal gravity, the products for the most part are isolated particles, quite variable in shape and ranging in dimension from about 70 to 2500 nm. Thus, many, although not all, of the particles are within the ultrafine definition. Under microgravity, the primary particles are nearly spherical, but they tended to agglomerate into large clusters, extending to lengths as great as 15 μm . The most unusual finding is that the degradation-product morphology is strongly dependent on PTFE insulation color in both environments. For example, white insulation is exceptional, producing isolated particles in both normal and microgravity. Other insulations (red, yellow, and black) yield aggregates in microgravity, but their shape and size are distinctly different for each color. These differences suggest that the degradation behavior is strongly influenced by possible minor changes in the polymer formulation. Confirmation of possible mechanisms awaits further testing.

Heat-transfer analyses were conducted to predict the temperature histories of the wires and particle plumes for normal gravity and microgravity. The predictions were verified by experimental temperatures, calculated from the wire power consumption and known copper resistivity. Predictions from the original analyses are not entirely satisfactory. A new modeling procedure is underway, using partial differential equations to couple the wire and the surrounding insulation temperature fields and accommodate phase changes and moving boundaries.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 0

TASK INITIATION: 5/94 **EXPIRATION:** 4/98

PROJECT IDENTIFICATION: 962-22-05-64

NASA CONTRACT NO.: NAG3-162

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

McKinnon, J.T., Todd, P.W., and Oberdorster, G. "Combustion of PTFE: The effects of gravity on ultrafine particle combustion." (CASI N96-30806) NASA CR 201112 (June 22, 1996).

Premixed Turbulent Flame Propagation in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Suresh Menon

Georgia Institute of Technology

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The overall objective of this research is to characterize the behavior of turbulent premixed flames and to use the experimental data to validate a novel computational method to simulate accurately the behavior of premixed flames. In order to understand the behavior of turbulent flames, access to all the length scales (from the device size to the Kolmogorov scale) in the flow field is required. A possible method to achieve this is to reduce the flow velocity. However, in normal-gravity this is not possible due to gravitational acceleration and the turbulent stresses are overwhelmed by buoyant stresses. Therefore, experiments in microgravity will be carried out that will allow the study of low-speed turbulent flames without buoyancy effects.

Task Description:

Premixed combustion of fuel-air mixtures will be studied in a Couette flow configuration which is essentially a flow between two parallel plates moving opposite to each other. The turbulent flow field will be characterized with the flame speed being the primary variable of interest. Additional data on pressure rise and temperature will also be measured.

Task Significance:

Improved understanding and modeling of practical turbulent flames will lead to increased efficiency and reduced pollutant formation. Practical applications of technology to industrial combustors and high throughput engines may be anticipated.

Progress During FY 1996:

The experimental study of cold Couette flow has been underway for sometime. Physically reasonable data for the mean flow profile have been obtained which clearly demonstrate that the flow field is turbulent. Measurements of the turbulence intensity have been affected by two problems: (a) the vibration of the belt and (b) the creation of an electrostatic field in-between the two Mylar sheets. Action is being taken to get rid of these effects.

The belt vibration is invisible to the naked eye. It is coupled with the belt speed and the belt tension, making it very difficult to assess. The belt flutter was determined by carrying out FFT of the velocity data and by measuring the local pressure field fluctuation. A characteristic frequency in the range 100-150 Hz was observed in the data which appeared to be affecting the velocity data. Furthermore, this fluctuation varies with belt speed and tension and thus, cannot be ignored since there is no way to quantify its influence by rescaling. To suppress the belt flutter it is planned to install plates on the outside of the belt so that the rigid surface can be used to damp the belt flutter. A similar strategy was employed in earlier studies in Sweden; however, the belt was quite long (> 1 meter) and therefore, initially it was felt that belt flutter may not be a problem with the shortened belt being employed in the Georgia Tech studies. However, recent data seem to suggest that this is a problem regardless of the belt length and needs to be removed. Once this problem is alleviated, detailed measurements of the velocity field including two-point correlation can be acquired in a reasonably short time since all the data acquisition systems are operational.

The electrostatic field appears to be generated by the friction of the Mylar belt on the metal rollers and is not discharged because the rollers are supported by a bearing whose oil layer tends to act as an insulator. To remove this problem it is planned to make the plates (noted above) of metal so that the plates will serve as grounding agents for the field. The fact that the "transparent" Mylar will be eliminated by using the metal plate is not considered a problem since v-velocity measurements are now being obtained by reorienting the laser beam at an angle so that it does not penetrate through the Mylar sheet.

The data acquisition for the cold flow is expected to be completed by October 1996.

As for the hot flow facility, the construction of the facility is nearing completion. Some delay was recently encountered due to the Olympics (the Olympics village was located at Georgia Tech) but the institute is now back to full operation. The hot facility is identical to the cold flow except for the absence of the moving belt and the use of stirring fans to generate turbulence. The facility has side walls that are made of high temperature resistant windows but these windows can be replaced by solid metal walls for later drop tests. This facility is needed to determine issues related to ignition and quenching control which needs to be automated and to obtain preliminary assessment of the ability to photograph the flame shape. This facility is to be completed by November 1996.

Numerical

The code for simulating this flow field is almost complete (including the option for reacting flows). The new method of subgrid mixing and flame propagation has been implemented in two 3D codes: a low Mach number incompressible code and a fully compressible code. The former code is computationally more efficient (since the time step is not limited by the acoustic speed); however, it can be used only for cases where the unsteady thermodynamic pressure is uniform in space (a condition that is reasonably approximated in the Couette facility) and for low to moderate heat release. It is planned to initially use this code to resolve the modeling issues and then move to the compressible code for the high heat release cases of realistic flames. Results for thin flame propagation (without heat release) have been recently reported in presentations.

Cases with heat release are currently being investigated and will be reported soon.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	1
PhD Students:	2	PhD Degrees:	0

TASK INITIATION: 5/94 EXPIRATION: 5/98

PROJECT IDENTIFICATION: 962-22-05-48

NASA CONTRACT No.: NAG3-161

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Menon, S., "Parallel simulations of unsteady turbulent flames." Proceedings of the 1996 EUROSIM International Conference HPCN Challenges: Parallel Simulation of Complex Systems and Large-Scale Applications", Delft, The Netherlands, Elsevier Science, to appear, 1996.

Presentations

Menon, S. and Chakravarthy, K., "Large-eddy simulations of turbulent premixed flames in couette flow." AIAA 96-3077, 32nd AIAA/ASME/SAE/ASEE Joint Propulsion Meeting, Orlando, FL, July 1-3, 1996.

Gravitational Influences on Flame Propagation through Non-Uniform Premixed Gas Systems

PRINCIPAL INVESTIGATOR: Dr. Fletcher J. Miller

Case Western Reserve University

CO-INVESTIGATORS:

Ross, H.D.

NASA Lewis Research Center (LeRC)

T'ien, J.

Case Western Reserve University

Task Objective:

The objective of this research is to determine the flame spread rates and flame spread character through non-uniform premixed gases (i.e., systems with a concentration gradient of fuel vapor perpendicular to the flame spread direction) in both normal and microgravity to determine gravitational effects. The induced flow ahead of the flame, as well as the redistribution of the fuel vapor layer caused by the flame will also be measured. An existing numerical model will be adapted to predict the measured quantities.

Task Description:

Flame spread through non-uniform gas mixtures will be studied in a partial enclosure in normal and microgravity. The gas mixture will consist of a layered system formed by diffusing either a pure gas or an evaporating liquid fuel from the floor of a long duct for a pre-determined length of time, resulting in a fuel vapor concentration gradient normal to the duct axis, and then igniting one end. Several diagnostics will be used to record the ensuing flame spread. Video cameras will observe the flame from the side to determine the flame shape and spread rate. A rainbow schlieren system will monitor the concentration gradients ahead of the flame and will be recorded on high-speed film. A laser absorption meter will also be used to make point measurements of fuel concentration ahead of the flame. The experiments will be conducted to determine the effect of initial fuel vapor concentration gradients as well as layer thickness, duct bottom material, oxygen concentration, and fuel type.

A secondary activity will be to adapt and further develop an existing numerical model (currently valid for flame spread over liquids) to predict the flow field and vapor layer redistribution caused by the flame. The model will be changed to handle the rapid flame spread expected here, and may also have some of the chemical reaction rate calculations improved.

Task Significance:

This research is of significant value in gaining a better understanding of flame spread through non-uniform mixtures which occur widely throughout combustion applications and unintended fires. Sprays, flame spread over liquids, and the leading edge of lifted turbulent diffusion flames are applications where flame behavior in layers is important. Compared with the two better known limiting cases [pure diffusion and pure premixed flames] these intermediate mixtures have so far received relatively little attention. This work should provide both new experimental data and models to understand flame propagation in such systems; this information would be readily useful to textbooks of the future. On the practical side, layered mixtures are ubiquitous in terrestrial fire hazards such as chemical spills, underground mining operations, and automobile and aircraft crashes. The flames in such systems have been shown to carry over fences, and to propagate past the ends of the fuel spill, thus representing a hazardous area beyond that associated with the original fuel location. They also represent a likely fire hazard aboard long-duration spacecraft such as the International Space Station -- perhaps second in probability only after electrical wire /insulation breakdowns -- since flammable gases may accumulate near waste storage, laboratory fluids, fuel cells, lasers, etc. Further research into these flames as proposed herein is essential to better understand this widespread phenomena, develop more robust models, and improve safety.

Progress During FY 1996:

This is a new project for 1996. We have begun design work on a drop rig for the 2.2 Second Drop Tower, and begun purchasing components. Some preliminary normal gravity experiments with liquid fuels have been conducted in a small enclosure, and a schlieren system was built to obtain images of the fuel evaporation prior to ignition. Test films of both flame spread and evaporation have been made using a high-speed cine camera. A hot gas tracer technique was used to measure the flame-induced motion in the gas. A full size fuel tray and duct have been designed and are in fabrication.

II. MSAD Program Tasks — Ground-based Research

Discipline: Combustion Science

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 0

TASK INITIATION: 8/96 EXPIRATION: 8/00

PROJECT IDENTIFICATION: 962-22-00

NASA CONTRACT No.: NCC3-

RESPONSIBLE CENTER: LeRC

A Fundamental Study of the Combustion Syntheses of Ceramic-Metal Composite Materials Under Microgravity Conditions - Phase II

PRINCIPAL INVESTIGATOR: Prof. John J. Moore

Colorado School of Mines

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective is to obtain an improved understanding of the effect of gravity on the combustion synthesis of 1) dense and 2) porous ceramic- and metal-matrix composites; develop new and improved materials and properties.

Task Description:

Combustion synthesis reactions are conducted both under normal gravity (various orientations of samples with respect to gravity) and microgravity conditions to generate either porous or dense ceramic composites in the presence of varying amounts of excess diluent, e.g. Al_2O_3 and/or excess liquid metal, e.g. liquid aluminum. The Al becomes liquid ahead of the propagating SHS reaction front and is available to fill residual pores in the ceramic matrix by capillary action, thereby resulting in a denser composite. On the other hand, for the synthesis of porous composites, the effects of gas generation during reactions on the porous matrix formation are being studied under different levels of gravity and partial pressure of the argon gas in the SHS reaction chamber. In a previous (Phase I) NASA grant, near-fully dense (95% relative density) dense composite materials have been produced using a one step, low cost simultaneous combustion-consolidation process. The microstructure and properties of the synthesized dense composite materials were also characterized and reported earlier, e.g., dense $\text{TiC-Al}_2\text{O}_3$ composites produced with a modulus of rupture of 300 MPa, and a fracture toughness (K_{Ic}) of 8 to 10 $\text{MPa m}^{1/2}$. The new (Phase II) grant is investigating the combustion synthesis of dense metal-matrix (greater than 50 volume % metal) composites with ceramic reinforcing particles that are either a) lighter than the metal matrix, i.e., $\text{TiB}_2\text{-Ni}_3\text{Ti}$, or b) heavier than the metal matrix, i.e., $\text{HfB}_2\text{-Al}$, in order to more clearly understand the effect of gravity in producing uniformly distributed ceramic reinforcing particles in a metal-matrix composite.

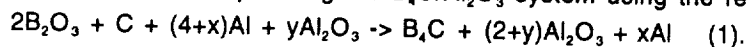
Task Significance:

An improved understanding of the role of gravity on the combustion synthesis of ceramic- and metal-matrix composite materials allows for new and/or improved synthesis techniques to be developed for these advanced composite materials that may exhibit improved microstructures and mechanical properties. One can also explore ways to develop brand new materials by microgravity processing (e.g. high surface area expanded or foamed ceramics, and fully dense interpenetrating phase composites). The expected benefits of such inexpensive, light, strong, and either highly porous or dense composite materials range from catalyst-support systems to high temperature and environmental filtering-systems (porous materials) to new lightweight materials that exhibit both high strength and toughness (dense materials).

Progress During FY 1996:

I. Porous Materials:

Prof. J. Moore has been pursuing the $\text{B}_4\text{C}/\text{Al}_2\text{O}_3$ system using the reaction:



The selection of this system is based on the observation that it showed expansions of approximately 150% under 2-g, and over 400% under 0-g conditions (Lear Jet), as opposed to 300% under n-g, after the combustion synthesis process. The student has concentrated her efforts on the more accurate control of the combustion temperature to avoid melting Al_2O_3 , with the expectation that, if successful, this would provide increased surface area in the expanded ceramic composite.

Two modes of combustion are being studied: 1) simultaneous, where the mixture is ignited by heating the whole pellet at once, and 2) propagating, where the ignition is at one end of the pellet. Depending on the value of y and combustion mode, the reactions are observed to be quenching, unstable, or stable, and the product has different pore

sizes, distribution and expansion.

Tania Mattor replaced Brooke Whitehead as an MS student. One of Tania's focus areas is the comparison of using either graphite or lampblack as the carbon source. She is also conducting the SHS reactions in the propagating mode under vacuum, near atmospheric and an intermediate subatmospheric pressure in order to more clearly understand the effect of chamber pressure in the synthesis of these porous ceramic materials. Under vacuum conditions both graphite and lampblack reactions proceed in an unstable spiral mode. If the power supply is turned off immediately after ignition, the reaction quenches out. However, if the power supply remains on until the reaction progresses partially through the pellet (i.e., preheating the sample), the reaction proceeds to completion in what appears to be a stable manner. Recorded combustion temperatures have varied between 1490C and 1886C if lampblack is used, and between 1545C and 2027C when graphite is used as the carbon source. Measured expansions so far have varied between 235% and 511%. Expansions under normal gravity but vacuum conditions can be even larger than low gravity but atmospheric argon conditions.

Tania's focus has been SHS reactions in the propagating mode using an excess $B_2O_3 + SiO_2$ mixture instead of Al or Al_2O_3 , i.e. $x=y=0$. The rationale behind this is that B_2O_3 is a gasifying agent, and it may be possible to produce additional porosity through an excess of B_2O_3 . SiO_2 is added to change the viscosity of the liquid B_2O_3 produced in the reaction prior to its gasification at higher temperatures reached in the SHS reaction. The B_2O_3 - SiO_2 excess was originally attempted at levels of 5 mole % and 10 mole %, but the 10 mole % samples melted and no reaction occurred. Of the 5 mole % samples there were two different ratios of SiO_2 to B_2O_3 examined (3% SiO_2 /97% B_2O_3 , the eutectic on the $SiO_2 - B_2O_3$ phase diagram (and providing a low liquid viscosity), and 50% SiO_2 /50% B_2O_3 , a composition having a considerably higher melting point than B_2O_3 (and, therefore, providing a high liquid viscosity).

For the 5 mole % excess of the SiO_2/B_2O_3 eutectic, combustion temperatures ranged from 1483 to 1764C, and expansions ranged from ~330 to 500% when graphite was used as the carbon source. When lampblack replaced graphite as the carbon source for the same system, observed combustion temperatures ranged from 1530 to 1938C with expansions ranging between ~380 to 460%.

For the 5 mole % excess 50% SiO_2 /50% B_2O_3 mixture, samples which utilized graphite as the carbon source exhibited combustion temperatures of 1545 to 1825C, and expansions of ~220 to 340%. The samples which utilized lampblack as the carbon source exhibited combustion temperatures of 1556 to 1774C and expansions of ~210 to 280%.

An interesting trend in combustion temperatures was noticed. As reaction chamber pressure was reduced from +22 psi (10 psi gauge) to +12psi (0 psi gauge), combustion temperatures increased. As the pressure is further reduced from 0 psi gauge to vacuum, the combustion temperatures decreased. The temperature decrease is attributed to the loss of B_2O_3 gas to the surrounding chamber with a corresponding decrease in reaction exothermicity. This speculation has been tested and confirmed using laser ablation ICP emission spectrographic analysis. The ratio of boron to aluminum (in the reacted pellet) was measured for all reaction pressures and the amount of boron with respect to aluminum was shown to decrease with decreasing chamber pressure.

Mercury porosimetry results have shown that bulk sample densities to date range between 0.4583 and 0.7053 g/cc for the foam compact, which placed the skeletal material density between 2.2382 and 3.0421 g/cc.

37 successful experiments were flown by Tania on DC-9 at LeRC in December, 1995. The microstructural and x-ray analyses as well as the search to determine the most useful method of porosity characterization are continuing. Tania had been using Hg porosimetry which yields a good characterization of porosity size and distribution for much of the sample, but the sample must be broken into small fragments prior to analysis and the maximum sample size is 0.17g. This results in eliminating much of the macroporosity in the sample and producing density measurements that contradict the linear expansion measurements. One does not expect to see much of a change in the total pore area measurements even when macroporosity is included in the calculation, but this will be confirmed via BET. If the BET and porosimetry values match well then Hg porosimetry will be used in the future to determine the microporosity (10-100 micrometers) characteristics, given the unavailability of a method that can account for both micro- and macroporosity characteristics.

Two NiTi experiments were attempted on DC-9 flights in December, 1995—one failed to ignite, the other ignited but only propagated a few millimeters before extinguishing. So far, several attempts in the lab by other students with NiTi reactions gave very poor results. Tania will try a few more reactions of her own before deciding as to whether it would be worthwhile to pursue producing porous NiTi with combustion synthesis.

Tania conducted another set of DC-9 flights in March and April, 1996 for a total of 39 successful completed runs out of 40 planned experiments. A few reactions did not register combustion temperatures, perhaps due to the amount of smoke produced and/or low temperature. Some cases were re-runs of the previous DC-9 flights last December as they did not report adequate data. Other additional cases included some 2-g data not gathered previously. SEM and x-ray analysis of the samples has started.

One new initiative resulting from her research will be to work with the Baylor College of Dentistry to see if they can use our porous materials for bone replacement applications.

II. Dense Metal Matrix Composite Materials:

Prof. Moore's request for international collaboration with GIL of Newfoundland, Canada, as part of his new NRA grant which started January, 1995, was approved verbally by Dr. Mickey King on the condition that no NASA money or facilities are used. The other MS student, Travis Woodger, went to Newfoundland in June, 1995 to conduct SHS experiments with acoustically levitated samples. His research objectives are to investigate the effects of gravity on the combustion synthesis of metal-ceramic composites during the generation of large amounts of one or more liquid products, i.e., greater than 50 volume percent liquid metal. He also intends to investigate the effect that gravity poses on the combustion synthesis process, product micro- and macrostructure, and the mechanical properties of the final composite. The two composite systems being investigated are 1) Al/HfB₂ and 2) Ni₃Ti/TiB₂ where the matrix component, i.e., Al and Ni₃Ti will exist as a liquid phase during processing. He has conducted thermochemical modeling of the two SHS reaction systems (i.e., TiB₂ ceramic particles in Ni₃Ti, and HfB₂ in Al).

Travis has returned from Newfoundland, where he has been working with Guigne International to conduct SHS experiments with acoustically levitated samples, in January 1996. The majority of his ground based experimentation has been completed. The results can be summarized as follows: 1) Composition Effects: There was a direct correlation between reaction propagation (wave) velocity and combustion temperature. For decreasing amounts of the ceramic phase (HfB₂ and TiB₂) there was an observed decrease in wave velocity and combustion temperature due to the diluent nature of aluminum and the less exothermic nature of the Ni₃Ti reaction; 2) Green Density Effects: The effects of green density for system 1 showed a strong correlation between wave velocity and combustion temperature. For system 2) a more complex relationship between wave velocity and combustion temperature was observed. An interesting observation made for this system was that at low green densities, ~45 percent of theoretical, a higher combustion temperature corresponded to a lower wave velocity; 3) Orientation Effects: Green pellets were reacted in three orientations. This included top, bottom, and horizontal ignition where the relationship between the wave velocity vector and the gravitational vector was 0, 90, and 180 degrees, respectively. A higher combustion temperature and wave velocity was observed for the bottom ignition samples. This is believed to be a result of increased heat transport by argon gas convection to the unreacted material resulting in preheating; 4) Microstructure: A marked effect of gravity on the distribution of the lighter (TiB₂ in Ni₃Ti) and heavier (HfB₂ in Al) ceramic reinforcing particles was observed. There was evidence of buoyancy induced TiB₂ segregation for system 2 as well as other possible gravity induced inhomogeneities in TiB₂ distribution. No inhomogeneities in microstructure were observed for system 1. This is probably due to the high viscosity of liquid aluminum.

Based on these results, the effects of gravity observed by Travis can be summarized as: 1) Preheating due to argon convection, resulting in higher combustion temperatures, 2) TiB₂ segregation, and 3) Inhomogeneity due to liquid Ni₃Ti convection.

Travis performed reduced gravity experiments using the DC-9 aircraft at LeRC at the end of April. The results of these experiments so far can be summarized as: 1) Densification Behavior: For system 1, the density of the final product was less under reduced gravity conditions than that observed for 1-g. The higher densities found to occur at 1-g are a result of the reacting pellet collapsing under its own weight when Al melts. For system 2, higher product densities were found for samples reacted under reduced gravity. The samples had higher densities due to the matrix phase remaining partially liquid for periods longer than the reduced gravity environment. Densification is probably

occurring during the high gravity phase of the reduced gravity trajectories. This high"-g densification is not an issue for system 1, because the period for which the sample remains liquid is less for this system, and the reacted samples are either completely or mostly solid (depending on concentration of reactants) during the high-g portion of the trajectory; 2) Combustion Temperature/Wave Velocity: For system 1, combustion temperatures were higher than those found in 1-g. Wave velocity measurements were similar to those measured under 1-g within experimental error with a large variability. Combustion temperature and wave velocity data were also higher for system 2 under reduced gravity. The higher temperatures and velocities are attributed to the absence of convective heat loss, even though the wave velocities under reduced and 1-g for system 1 were indistinguishable. These observations were true for all parameter variations of green density and volume fraction of the matrix phase.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0 BS Degrees: 0
MS Students: 3 MS Degrees: 1
PhD Students: 0 PhD Degrees: 0

TASK INITIATION: 1/95 **EXPIRATION:** 1/98

PROJECT IDENTIFICATION: 962-22-05-38

NASA CONTRACT NO.: NAG3-169

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Mattor, T., and Moore, J.J., "Self-propagating high-temperature synthesis of porous ceramics in microgravity." Experimental Methods for Microgravity Science, Annual TMS Conf., Anaheim, CA, February 4-8th, 1996.

Presentations

Mattor, T., and Moore, J.J., "Self-propagating high-temperature synthesis of porous ceramics in microgravity." Experimental Methods for Microgravity Science, Annual TMS Conf., Anaheim, CA, February 4-8th, 1996.

Mattor, T., and Moore, J.J., "Self-propagating high-temperature synthesis of porous ceramics in microgravity." Amer. Ceram. Soc. Conf., Indianapolis, IN, April 14-17th, 1996.

Stretched Diffusion Flames in Von Karman Swirling Flows

PRINCIPAL INVESTIGATOR: Dr. Vedha Nayagam

Analex Corporation

CO-INVESTIGATORS:

Williams, F.

University of California, San Diego

Task Objective:

The objective of this work is to investigate, both experimentally and theoretically, the effect of stretch on diffusion flames embedded in swirling flows. Theoretical models using asymptotic techniques (activation energy and rate ratio asymptotics) will be developed to interpret the experimental observations. Both the experiments and the theoretical models will be focused on the flammability boundaries in the low stretch and high stretch regimes.

Task Description:

The von Karman swirling flows are generated by spinning a fuel disk at different speeds. This geometry provides a unique way of establishing a desired stretch rate from very low to very high values. Also, the governing equations for this geometry reduces to a set of equations with only one dependent variable. A model with greatly simplified transport can thus be constructed, allowing for complex chemical and physical processes to be included at a fundamental level. Initial modeling effort will consist of activation energy asymptotics using a single-step chemistry with surface and gas-phase radiative heat losses. Later, rate ratio asymptotic models will be developed with a multi-step model for the gas-phase chemical kinetics.

As a part of this study detailed flammability maps for PMMA disks burning in O_2/N_2 environments at different pressures and a range of stretch rates will be generated. Experimental data on fuel vapor concentration profile, OH radical concentrations will be obtained using UV and IR sensitive CCD cameras. Critical strain rates at which soot formation ceases will be obtained by measuring flame radiation using a radiometer.

Task Significance:

The motivation for this study comes from the need to understand material flammability conditions in the slow convective environments commonly encountered in spacecraft environments. Here, flames that would normally extinguish on earth may be sustained. It is also hoped that the results obtained from studies of laminar-flame extinction may be applied for predictions in turbulent situations through estimates of strain rates in turbulent fields.

Progress During FY 1996:

An experimental apparatus capable of spinning a fuel disk at a specified angular speed ($0 < \Omega < 20,000$ RPM) has been built and integrated into a 2.2 Second Drop Tower frame. A graduate student (Matt King) from UCSD visited the NASA Lewis 2.2 second drop tower and performed preliminary calibration experiments using PMMA fuel disks in air. A preliminary model for a condensed-phase fuel burning in von Karman swirling flows has been constructed using activation energy asymptotic technique. Parametric studies are currently underway.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 0

TASK INITIATION: 8/96 EXPIRATION: 8/00

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NAS3-960

RESPONSIBLE CENTER: LeRC

Flow and Ambient Atmosphere Effects on Flame Spread at Microgravity

PRINCIPAL INVESTIGATOR: Prof. Paul D. Ronney

University of Southern California

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This program is a three-year experimental and theoretical study of the effects of ambient atmosphere on the properties of flame spread over thin and thick solid fuel beds. In particular the effect of the type of inert gas, which affects the Lewis numbers of fuel and oxidant, and the effect of the addition of sub-flammability-limit concentrations of gaseous fuels to the oxidizing atmosphere will be studied. The effect of convection will be studied through one-g and μ g experiments with and without a forced flow. Moreover, the influence of thermal radiation, whose effect is known to be markedly different depending on the convection level, will be addressed.

Task Description:

The emphasis of this study is on thermally thin fuels because of the limited μ g test time available in ground-based facilities. Preliminary scaling analyses suggest that thermally thick fuels can be examined as well when gaseous fuel is added to the oxidizing atmosphere.

The experiments will be conducted in a combustion chamber in which a convective flow of a few cm/sec can be imposed in the direction opposite the flame spread. The oxidizing atmosphere will be mixed by the partial pressure method. For tests of Lewis number effects, inert gases He, Ne, N₂, CO₂ and SF₆ will be used since they provide Lewis numbers from about 0.3 to 1.4. CO and CH₄ will be used for the gaseous fuels. Thin fuel samples will be ashless filter paper and thick fuel samples will be PMMA. Fuel samples of varying thickness will be ignited by the heat generated by a current passed through a coiled nichrome wire coated with nitrocellulose.

The primary diagnostics are video and an array of fine-wire thermocouples to measure the temperature simultaneously at several locations. The video records provide information on the spread rate and flame shape. The thermocouples give an independent check of the spread rates and the existence (or lack thereof) of a separate flame front in the case of added gaseous fuel. The temperature data may also be used to determine the heat flux from the gas phase to the fuel bed, which can be related to the spread rate.

Task Significance:

The understanding and control of accidental fires is a critical safety issue in both terrestrial and space-borne environments. The proposed work would provide insight that could be used to assess the fire hazards associated with non-standard atmospheres that might be employed in future manned spacecraft. Also, fires in enclosures produce a considerable amount of unburned vaporized fuel and partially combusted gases such as CO. One-g experiments have shown that the addition of combustible gases such as CO to the oxidizing atmosphere may increase the flame spread rate substantially. This study could provide information to improve models of fire development and spread in enclosures at one-g and μ g.

The influence of weak forced convection is particularly important for studies of flame spread at μ g because there is very little buoyancy-induced flow at μ g. Experiments by Olson and collaborators shows that the presence of forced convection currents (for example due to ventilation systems in manned spacecraft) can have a profound effect on the spread rate and extinction conditions. Consequently, the understanding of these effects is critical to understanding how fires might start, spread, and be extinguished at μ g conditions.

Progress During FY 1996:

Microgravity experiments in the NASA Lewis 2.2 Second Drop Tower have been initiated. The previously built apparatus has operated successfully and has yielded some interesting results on the effects of adding gaseous fuel (CO or CH₄) to thin solid fuel (kimwipes). It was found that this added gaseous fuel increased the flame spread rate of the thin solid fuel significantly more in microgravity conditions than in 1g conditions. Video from a CCD and

an Interferometer were compared to get both qualitative and quantitative data. It can be seen that for low gaseous fuel concentrations the flame spread rate is lower at microgravity, which is consistent with earlier data by Olson and others in atmospheres without gaseous fuel, increasing the gaseous fuel concentration raises the microgravity flame spread rate disproportionately to the 1g spread rate increase. During the NASA LeRC campaign many sets of data were taken to determine what compositions would yield the most valuable data. Additional 2.2 Second Drop Tower testing was conducted in July and August to continue this research, and preliminary results indicate very interesting diluent/Lewis number effects where flame spread in a quiescent microgravity environment is actually faster than in normal gravity.

The effect of gravity on upward spreading flames was also discussed in an earlier report. It was found that the experimental flame spread results agreed well with the scaling predictions outlined earlier. However, it was found that the pressure effects needed to correlate each set of data needed further work. It was found that certain diluents, pressures, and sample widths produced flames that were roughly the size of the chamber. Therefore a new taller chamber was built and used. The results of the additional tests done in this chamber were found to correlate well with the old chamber. Nitrogen, Carbon Monoxide, Sulfur Hexafluoride, and Helium were each used as diluents and the oxygen concentration, sample width, pressure, and sample thickness were varied. We are analyzing the results and further 1g tests may be conducted if deemed necessary.

Finally, new chambers are being designed for experiments to be done at 1g and microgravity with forced flow environments. The scaling analysis developed by the PI and discussed in previous reports also included forced flow environment situations that will be compared to the results obtained experimentally with these new chambers.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 2
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/94 EXPIRATION: 4/98

PROJECT IDENTIFICATION: 962-22-05-61

NASA CONTRACT No.: NAG-3-16

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Honda, L. and Ronney, P.D., "Mechanisms of concurrent-flow flame spread over thin solid fuels." presented at the Fall Technical Meeting of the Western States Section of the Combustion Institute, Stanford, CA, October 30-31, 1995.

Ronney, P.D. "Combustion experiments in space." 36th Israel Annual Conference on Aerospace Sciences, Haifa, Israel, February 21-22, 1996.

Flammability Limits and Flame Dynamics of Spherical Flames in Homogeneous and Heterogeneous Mixtures

PRINCIPAL INVESTIGATOR: Prof. Paul D. Ronney

University of Southern California

CO-INVESTIGATORS:

Niioka, T.

Tohoku University

Task Objective:

The objective of this work is to study homogeneous and heterogeneous spherical flames in microgravity. Both types of flames have fundamental similarities which make it advantageous to study both in the same microgravity environment. The following sub-tasks are scheduled to be pursued:

- (1) Study of homogeneous combustion in premixed gases near the lean flammability limit.
- (2) Study of heterogeneous combustion in aerosols near the lean flammability limit.

Task Description:

For task 1, we are studying premixed gas mixtures that produce quasi-steady or fully steady flames in the JAMIC facility. The mixtures to be studied complement those to be flown on the space shuttle in the Structure of Flame Balls at Low Lewis Number (SOFBALL) experiment.

For task 2, we are studying heterogeneous mixtures of fuel aerosols that produce quasi-steady spherical flames.

Task Significance:

The results will lead to an improved understanding of homogeneous and heterogeneous combustion that produces spherical flames in microgravity. The homogeneous gas study will form a complementary study to a space experiment. Heterogeneous combustion occurs in many practical combustion devices and is not well understood because of the effects of buoyancy on flame propagation and extinction limits.

Progress During FY 1996:

1. Study of homogeneous combustion in premixed gases near the lean flammability limit.

A set of microgravity experiments were performed in the JAMIC drop tower using weakly combustible gas mixtures having low Lewis number. These mixtures were chosen because prior drop-tower and aircraft experiments have shown that these mixtures exhibit flame balls. The JAMIC facility provides a much longer microgravity duration than other drop-tower facilities and much higher quality microgravity than aircraft experiments. The data obtained can thereby be used to extend prior ground-based experiments and augment space flight experiments to be performed on CM-1/SOFBALL. The mixtures were ignited in the center of a 20 cm diameter cylindrical chamber 20 cm in length with an electric spark of typically 2 J energy content. The resulting flames were observed with various combinations of direct color video, intensified monochrome video, interferometry, thermocouples, a chamber pressure transducer, and a radiometer.

Preliminary data indicate that the test results are very consistent with prior aircraft microgravity results despite the much poorer quality of microgravity in the aircraft experiments. This result is somewhat surprising considering that our estimates suggest that in the aircraft experiments the gravity levels are still large enough that transport of heat and mass to and from the flame balls are likely to be dominated by buoyant convection rather than diffusion and radiation.

Both sets of experimental data show larger flame balls and weaker radiant emission than theoretical predictions. This result is also somewhat surprising because radiant emission should increase with increasing flame ball size, thus the directions of the discrepancies seem contradictory. The simplest explanation would be that the radiative model employed in the calculations over predicts the actual loss, however, there is no apparent reason to doubt this well-established and widely-used radiation model.

One unusual feature of the experiments was that the flame balls in hydrogen-air mixtures were extremely stable whereas in the carbon dioxide and sulfur hexafluoride-diluted mixtures the flame balls have a noticeable tendency to drift even at the very low g-levels in the JAMIC facility. This raises the intriguing possibility that there is yet another radiation-driven instability (since the sulfur hexafluoride and to a lesser extent carbon dioxide mixtures are optically thick) that causes these flame balls to develop a drift velocity. If the drift were simply a gravity effect, it should occur also in the hydrogen-air tests.

2. Study of heterogeneous combustion in aerosols near the lean flammability limit.

No results reported to date on Prof. Niioka's studies.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 4/96 EXPIRATION: 4/97

PROJECT IDENTIFICATION:

NASA CONTRACT No.: NAG3-181

RESPONSIBLE CENTER: LeRC

Combustion Research

PRINCIPAL INVESTIGATOR: Dr. Howard D. Ross

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:No Co-I's Assigned to this Task

Task Objective:

The task objective is to advance the understanding of fundamental combustion phenomena and/or processes that are affected by the presence or absence of gravity.

Task Description:

The research approach is to provide for limited precursor studies by external investigators and for the engineering and fabrication of hardware needed to conduct in-house research and assist in the research efforts conducted on-site at LeRC in support of Code UG-sponsored Principal Investigators (PI's) and National Research Council (NRC) graduate student researchers. Funds for facility overhead charges are provided through separate Research and Technology Operations Plans (RTOP) resources.

Subtasks are funded in part by this task, or are included for completeness at the request of NASA Headquarters.

Task Significance:

Significance varies with the various research efforts, and therefore, more focused, effort-specific, statements are given below.

Progress During FY 1996:**Objective:**

To measure full field flame temperatures under a variety of environmental conditions. This includes variations in pressure, oxygen concentration, and g-level. Some of these flames will be near the extinction limit and the measured temperature profiles will be compared to previously published numerical results.

Approach:

An interferometry system is being used to take these full field flame measurements. This type of optical measurement has advantages over standard thermocouple based measurements, as it is non-invasive and can provide a two-dimensional temperature field for the entire flame at a specific instant in time.

Initial tests are being conducted in normal gravity using the temperature profile generated by a heated vertical flat plate. The temperature profile for this case is presented in the scientific literature and is well known. The optical measurement will be compared to the published temperature profile.

Significance:

Current theories detailing extinction of flames due to quenching predict a reduction in the gas-phase temperature. This technique will allow flame temperature measurements to be taken to examine these theoretical and numerical predictions.

In addition, this technique could be applied to other situations in which full field flame temperature are required.

Progress:

The post-doctorate program was started on July, 11, 1996. The delay in the start date was caused by delays in completing dissertation research at Case Western Reserve University.

The optical system being used is hardware from the Laminar Soot Processes Experiment that has been used to measure soot volume fractions. The de-collimating portion of the optical hardware is modified to accommodate a diffraction plate at the focal point of the light beam. This diffraction plate is the critical element in the PDI (Point Diffraction Interferometer) system, and it produce fringes in the beam that can be used to measure changes in the

index of refraction of the gas that the laser beam is passing through. This interferogram is recorded by a video camera for viewing and storage on a video cassette. A new vertical translation stage was machined at NASA Lewis for the PDI unit, which will allow for better positioning of the plate in the focal point of the laser beam. A combustion chamber was manufactured and assembled for normal gravity experiments at a variety of pressure and gas compositions. An internal NASA Lewis safety permit was acquired for the normal gravity experiments.

A computer was set up in the laboratory for use with this experiment. The computer is equipped with a frame grabbing board and associated software. This will allow images to be grabbed from the video camera for later analysis.

Current efforts are focused on stabilizing the fringes produced by the system. Vibrations from the surrounding lab area, including the lab floor are disturbing the optical hardware. A set of vibration dampers was ordered for the hardware with delivery due in September.

Once the fringes are stabilized, the optical measurements must be calibrated. Optical temperature measurements of the thermal boundary layer from a heated vertical flat plate will be compared to the known analytic solution. The hardware (mechanical and electrical) required for this calibration is currently being assembled.

A secondary task underway is an analysis of microgravity flame spread rates from interacting flames. The test parameters included pressure, gas composition, and sample separation distance. These experiments were conducted previously under the direction of Dr. David Urban (NASA Lewis). The spread rate data will be used in conjunction with flame temperature measurements taken with the interferometry hardware.

Sub Objective:

Measure the shapes and model the structure of microgravity laminar gas jet diffusion flames.

Sub Approach:

The initial focus involves enhancements in a NASA LeRC General-Purpose Combustion Rig for investigation of microgravity laminar gas jet diffusion flames in the NASA 2.2-Second Drop Tower. The rig will be used to obtain flame shape data for comparison to existing models of microgravity jet diffusion flames.

Sub Significance:

This research will contribute to current understanding of microgravity diffusion flames, guide flame selection in future experiments, and test the laminar flamelet concept for microgravity flames. Thus the research should prove significant to both combustion science and microgravity fire safety.

Progress:

The plumbing in this rig was modified so as to minimize the ignition flash and fabricated a retracting-wire ignitor which provides reliable ignition with minimal disturbance. Optimization was also completed for the CCD camera configuration and added a CH-line filter for ideal imaging of the flame sheet.

Following these modifications, flame shape data was obtained for methane and ethane diffusion flames (this with the assistance of a NASA/OAI summer intern). Present operating conditions cover a broader range of fuel flow rates, chamber pressures and burner diameters than previous microgravity studies. We have correlated the methane and ethane flame lengths with Reynolds number in agreement with the theory of Roper (Combust. Flame, 29:219, 1977). We have found that previous studies reported flame lengths which are longer than present measurements, probably due to interference in those earlier studies from soot luminosity and carbon-dioxide afterglow. We have also correlated flame width with Reynolds number, but the correlation is weaker than that for flame length.

In tandem with these experiments, Dr. Sunderland has been developing a computational model of microgravity laminar gas jet diffusion flames using the TEACH code and state relationships.

In a separate effort, he has also been supporting the LSP flight experiment, particularly with the mounting and examination of transmission electron microscope grids.

As a follow-up to work he performed last year at the University of Michigan under the direction of Professor G. M. Faeth, he assisted with a paper that was accepted for publication in Combustion and Flame. Dr. Sunderland presented a related paper at the Central States Combustion Institute meeting in St. Louis and a related work-in-progress poster at the prestigious 26th Intl. Symposium on Combustion.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 1/91 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-22-05-08

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Ross, H. "Measurements and predictions of soot formation in laminar premixed flames." Spring Technical Meeting of the Combustion Institute central States Section, St. Louis, MO, May 6, 1996.

Ross, H. "Soot formation in laminar premixed ethylene/air flames at atmospheric pressure." (Poster presentation) 26th Symposium on Combustion, The Combustion institute, Naples, Italy, July 30, 1996.

Combustion of Unconfined Droplet Clusters in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Gary A. Ruff

Drexel University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to study the combustion of well-characterized drop clusters to better link isolated droplet and droplet array studies with those involving spray flames. In this study, which will be conducted in a series of drop tower experiments, the formation of the drop clusters will be precisely controlled using an acoustic levitation system so that very dilute, as well as very dense clusters can be created and stabilized before combustion is begun. Tasks to be accomplished during this research include (1) the design and fabrication of a unique droplet combustion experiment using acoustic levitation to stabilize a droplet cluster prior to combustion, (2) investigation of droplet combustion in the individual particle combustion, group combustion, and sheath combustion regimes by varying the number of droplets, droplet size, and cluster diameter, and (3) investigation of the effect of drop size distribution, droplet composition, and continuous-phase oxygen concentration on cluster combustion.

Task Description:

The first step in achieving these objectives will be to construct an apparatus in which a cloud or cluster of drops is formed while being levitated in an acoustic resonance chamber prior to combustion in microgravity. Using one or more droplet-on-demand drop generators, the number and size of the drops in the cluster can be accurately controlled. A small electrical charge will be placed on the drops to prevent coalescence during the formation of the cluster. The size and shape of the cluster can be controlled through the design of the acoustic resonance chamber and selection of the resonance frequency. Additionally, group combustion numbers (ratio of the mass transfer between the phases in the cloud to the mass transfer between the ambient and the cloud surface) between 0.1 and 100 can be obtained which encompasses the individual particle combustion, group combustion, and sheath combustion regimes. Because the presence of an acoustic field greatly influences drop combustion, the field will be turned off at the start of the microgravity period. The resonance chamber and drop generators will also be retracted from the cluster so that they do not interfere with the combustion process.

The diagnostic capability to be incorporated into the experimental package includes multiview imaging to view the motion of the droplets and LIF to view the position of the flame front. Light sheet visualization will also be used to obtain a different perspective of the motion of drops in the cluster. Continuous-phase temperature histories in the drop cluster will also be obtained using micro-thermocouples suspended across the cluster. Because the test facility will be designed with optical access for cameras, other diagnostic techniques being developed in the NASA Microgravity Science and Applications program for use in drop towers can be incorporated into the experiment as desired.

Initially, droplet clusters will be formed using n-decane, heptane, and methanol, as many of the droplet array and group combustion studies have done. This will allow the droplet burning rates obtained from this research to be directly compared with results of isolated droplet and droplet array studies. The position and movement of the flame front will provide some of the first experimental data for comparison with group combustion models obtained using large numbers of drops. Data will be obtained as a function of group combustion number, drop size, number of drops, drop size distribution, and ambient oxygen concentration. Several tests are also planned in which drops will be formed with binary fuels composed of heptane/methanol, heptane/ethanol, or heptane/hexadecane to experimentally investigate the effect of fuel volatility on cluster combustion and help define future research. These fuel compositions are the same as those used in other drop combustion research, immediately linking the current results to existing research.

Task Significance:

Isolated drop and drop array studies have become common methods to isolate and investigate the many complexities of the drop combustion process. Accordingly, several isolated drop, drop array, and spray studies are currently in progress under the NASA Microgravity Science and Applications program. Results from these research programs

indicate that even with the effects of buoyancy removed, the extrapolation of the results from droplet array studies to spray flames is difficult. The problem arises because even the simplest spray systems introduce complexities of multi-disperse drop sizes and drop-drop interactions, coupled with more complicated fluid dynamics.

Not only do these features make the interpretation of experimental data difficult, they make the problem very difficult to analyze computationally. Group combustion models have become a popular method to investigate the behavior of large numbers of interacting droplets. In these models, the interaction between droplets is treated in a statistical manner rather than tracking and evaluating drop interactions using a Lagrangian approach. These models have allowed very comprehensive investigations of the combustion of multi-component drops, spray ignition phenomena, high-pressure combustion, *etc.* While these models idealize actual spray systems to a point where they can be treated computationally, the experimental analogy to these models is difficult to achieve. Therefore, even though these models have provided useful results, the verification of the results with direct comparison with experimental data is still lacking.

Direct experimental measurements in well-defined droplet clusters would fill a large gap in our current understanding of droplet combustion. The results of this study will provide an intermediate link between droplet array studies and those performed using full combustor spray systems. They will also provide unique experimental data for the calibration, verification, and improvement of group combustion models that are currently being applied to complex flow situations.

Progress During FY 1996:

The proposal for this project was approved in March 1996 and the project began on June 1, 1996. The project team consisting of the PI, a post-doctoral research assistant, and two graduate students has been assembled. The design of the two major components of the experimental facility, namely the droplet-on-demand generators and the acoustic levitation device is progressing.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-22-00

NASA CONTRACT No.: NAG3-188

RESPONSIBLE CENTER: LeRC

Reduced Gravity Combustion with 2-Component Miscible Droplets

PRINCIPAL INVESTIGATOR: Prof. Benjamin D. Shaw

University of California, Davis

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Determine the combustion of two-component miscible droplets in reduced gravity via experimental and theoretical analysis. Specific objectives were to gather data on transient liquid behaviors (e.g., diameter histories and disruption), transient flame behaviors (e.g., sudden flame contraction and extinction), and sooting (e.g., luminosity and transport of observable soot particles).

Task Description:

The experiments involved burning two-component miscible droplets in environments of differing pressures and compositions. Data was obtained by direct photography of droplets and flames. Droplets initially about 1 mm in diameter and with components that differ significantly in volatility were studied.

Hydrocarbon (e.g., heptane/hexadecane) or alcohol mixtures in oxygen mole fractions from about 0.1 - 0.5 and initial pressures from 0.5 - 2 atm were used. Different inerts in the gas phase enhance or inhibit certain phenomena; e.g., CO₂ inhibit soot formation, while helium may promote extinction by increasing gas transport rates. Theoretical and computational research includes: modeling of fundamental droplet combustion phenomena; studies of allowable acceleration levels and durations to define experiment requirements; and studies of issues such as allowable droplet oscillation amplitudes, oscillation decay times, and pre-ignition vaporization.

Task Significance:

The reduced gravity experiments should yield insight into the efficiency of liquid-phase species diffusion, since this diffusion may markedly influence combustion behaviors (e.g., two-staged combustion behaviors). By noting times for flame contraction to occur, calculations for effective liquid-phase species diffusivities may be made (e.g., with asymptotic or with numerical models). Finally, unique sooting behaviors may appear since gas-phase compositions may differ significantly with time. Differences in sooting may be observable photographically by noting behaviors of apparent flame luminosities and soot particles large enough to be observed.

The theoretical efforts will aid interpretation of the reduced-gravity experiments as well as improve understanding of fundamental phenomena that occur during combustion in reduced-gravity.

Progress During FY 1996:**Experimental**

A new droplet combustion apparatus developed and built at the University of California, Davis was used for a large number of experiments. Use was made of the 2.2 Second Drop Tower at the NASA Lewis Research Center. From August 1994 to February 1995, 133 successful drop tower experiments were performed (out of 203 attempts). Ambient pressures were varied from 0.3 - 3 atm (abs), the diluents N₂, CO₂, Ar and He were used, and many different fuel mixtures (alkanes and/or alcohols) were investigated. The primary fuel mixtures studied were heptane/hexadecane, in air or O₂-He environments. About 40 experiments were conducted with heptane/hexadecane mixtures in O₂-He environments at 1 atm or below. The experiments were very successful, allowing many new phenomena to be observed as well as providing verification of theories related to flame contractions associated with combustion of two-component droplets.

We are now in the process of analyzing the films from these successful experiments. Because of the large volume of data obtained, this process has taken several months; the data analysis will be completed this fall. An overview of the experimental results can be found in Ref. [1]. Results have indicated that liquid-phase species diffusivities (as estimated by noting times for flame contractions) varied significantly with the ambient pressure. As the ambient pressure was increased, values for effective liquid-phase species diffusivities increased as well. This is most likely

related to the fact that droplet surface temperatures will increase with increasing pressures, which will increase liquid species diffusion rates. Burning rates, transient flame behaviors, extinction, and visible sooting behaviors varied strongly with ambient gas pressure and composition, as well as with the initial droplet diameter and initial droplet composition. Articles on these (and other) aspects of the experiments have been submitted for publication [2-5].

Computational:

Detailed computational modeling (in collaboration with Professor H.A. Dwyer) has focused upon predicting effects of capillary flows on transient droplet vaporization. A finite-volume method is used, and variable properties are allowed in the liquid and gas phases. Modeling of single-component droplet vaporization in a hot environment has clearly shown that capillary flows dramatically influence droplet vaporization and internal circulation behaviors under conditions representative of slowly-drifting droplets in reduced-gravity experiments as well as rapidly-translating droplets in practical high-pressure sprays (see [6] and the references contained therein).

The computer code was recently modified to allow for multicomponent liquids. Thermal and solutal Marangoni effects on transient droplet gasification are now being investigated.

Analytical:

To aid interpretation of experimental efforts, analytical studies of gasifying droplets in reduced-gravity environments have been performed. These efforts focused on determining: (1) effects of small gravitational levels on droplet gasification; (2) and hydrodynamic stability of two-component droplets. Each effort has considered evaporation; combustion will be considered later.

The gravity-level research [7] focused on how small gravitational levels affect droplet gasification characteristics. The (viscous) conservation equations were nondimensionalized, and a small parameter that accounts for the effects of gravity was identified. Asymptotic analyses were developed in terms of this parameter. Near a droplet, the flowfield is spherically symmetric to leading order. Outer zones exist, however, where buoyancy significantly influences the flow; a stagnation point is predicted to exist in an outer zone.

The stability analyses [8,9] addressed the problem of predicting when spherically-symmetrical gasification of two-component droplets can be expected to be hydrodynamically unstable from surface-tension gradients. It was found that with zeotropic mixtures and for $\partial s/\partial T < 0$ and $\partial s/\partial T < 0$ (where s is surface tension, T temperature, and y the liquid mass fraction of the more volatile droplet component), the thermal Marangoni effect is stabilizing and the solutal Marangoni effect is destabilizing. Heptane/hexadecane mixture droplets were predicted to be hydrodynamically stable. For methanol/water droplets, there is a critical radius for stability. When a droplet is initially pure methanol and absorbs water from the ambient, the critical radius depends upon the relative humidity of the environment. The instability for water/methanol droplets stems from the fact that water has a very high surface tension relative to methanol.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	1
PhD Students:	2	PhD Degrees:	0

TASK INITIATION: 8/91 EXPIRATION: 3/96

PROJECT IDENTIFICATION: 962-22-05-39

NASA CONTRACT NO.: NCC3-245

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Aharon, I. and Shaw, B.D. "Combustion of heptane/hexadecane mixture droplets in reduced gravity at sub-atmospheric, atmospheric and elevated pressures." Western States Section of the Combustion Institute, Fall meeting, Stanford, CA., paper #WSS 95F-226, November, 1995.

Aharon, I., Shaw, B.D., "Marangoni instability of bi-component droplet gasification in reduced gravity." Western States Section of the Combustion Institute, Fall Meeting, Stanford, CA, paper #WSS 95F-227, November, 1995.

Aharon, I., Shaw, B.D., Gage, J.J., Jenkins, A.J., and Kahoe, T.J., "Combustion of alcohol mixture droplets in reduced gravity." Western States Section of the Combustion Institute, Fall meeting, Stanford, CA, paper #WSS 95F-228, November, 1995.

Quantitative Measurement of Molecular Oxygen in Microgravity Combustion

PRINCIPAL INVESTIGATOR: Dr. Joel A. Silver

Southwest Sciences, Inc.

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

There are two objectives of this task. First is to develop diagnostics based on diode laser absorption spectroscopy for use in microgravity combustion research. The general technique is expected to be applicable to major gases involved in combustion and in spacecraft cabin environments. The specific application in this task is to the quantitative determination of molecular oxygen. The second objective is to develop a better understanding of the relative roles of diffusion and reaction of oxygen in microgravity combustion. Oxygen has a major role in controlling flame properties such as flame front speed, extinguishment, flame size, and temperature.

Task Description:

This investigation involves the determination of molecular oxygen using diode laser absorption spectroscopy. This technique uses a compact, low power optical system to probe the near infrared bands of oxygen. Though these bands are relatively weak, high sensitivity is maintained by means of wavelength modulation of the diode laser with detection at twice the modulation frequency. A compact laser scanner permits the laser beam to traverse the entire flame region. This scanner eliminates the need to use optical fibers in the setup. A compact electronics package includes all control, detection, and data acquisition electronics.

Task Significance:

Oxygen, as the primary oxidizer in flames, controls the major flame properties such as flame spread, flame front speed, temperature, and extinguishment properties. Its quantitative determination therefore is necessary both for an improved understanding of flame behavior in general and for fire safety on board spacecraft. Oxygen measurement is also critical for ground-based applications such as engine efficiency, energy production, air quality monitoring, and industrial processes such as steel manufacture. The specific technique under development is a compact, lightweight, and rugged instrument offering a wide range of laboratory, field, and industrial process measurements.

Progress During FY 1996:

Additional features were added to the data analysis program for calibration of the O_2 concentration at each position and time. The calibration is done by fitting a measured, ambient O_2 spectrum over a known path length to a synthetic spectrum at the known value of pressure, temperature, path length, and modulation index.

The fitting routines were modified to permit more rapid fitting by using pre-computed spectra to determine a best temperature and then solving the linear problem for concentration.

Software development was essentially completed. Two methods were provided for data analysis: (1) a least squares determination for concentration is made from predetermined theoretical spectra at 18 temperatures ranging from 300 to 2000 K; best temperature is determined from minimum value of chi squared vs T; finally a linear fit is done to the experimental data to determine final mole fraction; and (2) Fourier transforms are computed to directly convert the 2f spectra to absorption lineshapes, and then linear fitting methods are used to determine T and mole fraction. For both methods an in situ calibration is provided by the known ambient O_2 concentration.

Spectra of O_2 in a diffusion flame were recorded using a slot burner.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/94 EXPIRATION: 6/97

PROJECT IDENTIFICATION: 962-22-05-51

NASA CONTRACT NO.: NAS3-265

RESPONSIBLE CENTER: LeRC

Numerical Modeling of Flame-Balls in Fuel-Air Mixtures

PRINCIPAL INVESTIGATOR: Prof. Mitchell D. Smooke

Yale University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The overall objective of the proposed work is to understand if and the mechanisms by which stationary, spherical flames, sometimes called flame balls, stabilize in a quiescent, premixed gaseous fuel-oxidizer environment. These flames have been observed experimentally shortly after ignition in microgravity, but their long-term persistence is as yet undetermined.

Task Description:

Combustion models that simulate pollutant formation and study chemically controlled extinction limits in flames often combine detailed chemical kinetics with complicated transport phenomena. One of the simplest models in which these processes are studied is the plane premixed laminar flame. This problem is appealing due to its simple flow geometry and it has been used by kineticists in understanding elementary reaction mechanisms in the oxidation of fuels. Although premixed flames have been studied extensively (experimentally and numerically) in a normal Earth based gravity environment, there is relatively little experimental and virtually no numerical investigations of these systems in a microgravity environment. To this end, we have begun a program designed to study computationally the effects of radiation losses on spherically symmetric premixed hydrogen-air flames in a microgravity environment in which there are no convective flows. We are considering a detailed transport and finite rate multistep kinetics model. To be able to compute solutions (both stable and unstable) in the neighborhood of the lean and rich extinction limits, we must modify the basic solution algorithm to include an arclength continuation procedure. In this way a parameter such as the equivalence ratio can be varied while still having a computationally stable algorithm.

Task Significance:

The significance of this effort is to enhance the understanding of very basic combustion phenomena, such as flammability limits and stabilization mechanisms, integral to many combustion technologies.

Progress During FY 1996:

During the first two years of the project our goals have included verifying the sensitivity of the flame ball radius and the value of the lean and rich flammability limits to 1) the hydrogen-air chemistry, 2) the transport model, 3) the radiation approximation, 4) the length of the computational domain and 5) the far field radiation losses. Our early hydrogen-air flame ball computations [1] employed a Curtiss-Hirschfelder transport approximation with a radiation model in which interpolated emissivity data was used to construct an approximation for the divergence of the radiative heat flux on a fairly small domain.

Transport

Utilizing the kinetic theory of dilute gas mixtures, we can write the following expression for the species diffusion velocities

$$V_k = -K \sum_{k=1}^K D_{k1} - X_1 - q_k - \log(T)$$

where D_{k1} , $1 \leq k, 1 \leq K$, are the species diffusion coefficients and q_k , $1 \leq k \leq K$, are the thermal diffusion coefficients.

The species diffusion coefficients are symmetric and satisfy the important relations

$$\sum_{k=1}^K Y_k D_{k1} = 0, \quad 1 \leq 1 \leq K, \quad \sum_{k=1}^K Y_k q_k = 0$$

which guarantee the mass conservation constraint

$$\sum_{k=1}^K Y_k V_k = 0$$

Using the recent theory of interactive transport algorithms [2], rigorous kinetic theory expressions can be derived for all of the transport coefficients. In particular, the thermal conductivity, the diffusion coefficients, and the thermal diffusion coefficients are obtained by solving constrained singular linear systems. These approximate expressions are accurate and computationally much more cost-effective than a direct numerical inversion of the associated linear systems. Moreover, the approximate species diffusion coefficients and thermal diffusion coefficients automatically satisfy the mass conservation constraint (3).

Radiation

Since radiation plays a key role in defining the structure and stability of flame-balls, it is necessary to construct a careful estimate of the radiation term q_R . We assume that for hydrogen-air mixtures the only significant radiating species is H_2O (For methane-air systems additional terms from CO and CO_2 will be included). By utilizing an optically thin limit in which self absorption of radiation is neglected, the divergence of the net radiative flux is given by

$$(1/r^2) (d/dr(r^2 q_R)) = 4\pi \sum_i a_i B_i(T)$$

where $B_i(T)$ is the Planck function evaluated at the band centers of the contributing vibration-rotation or pure rotational bands whose integrated intensities are given by a_i [3,4].

Computations

Utilizing a modified hydrogen-air reaction mechanism [5] with the transport model employed in [1], we continued our studies from last year in which flame balls were computed as a function of the equivalence ratio f . Temperature and radii results were compared with our original computations. While the temperature and the size of the flame ball at the rich limit show only minor changes, there is a modest increase in the rich flammability limit with the new mechanism. Only very small changes occur on the lean side but they move in the direction of increased agreement with the experiments [1]. We have also compared the temperature and radii as a function of the equivalence ratio for the new mechanism/old transport calculations with calculations made with the new mechanism and the transport and radiation models discussed above. Essentially no major differences were found. Nevertheless, due to its more accurate formulation, the detailed transport and band radiation models will be utilized in all future flame ball calculations. More recently, we examined the effect of far field radiative losses due to water vapor. By including various percentages (mole fraction) of water vapor in the far field mixture, we have been able to predict modest changes in the lean flammability limit of the flame balls. Work in this area is continuing in collaboration with University of Illinois Professor, John Buckmaster. Future work will examine the structure of hydrogen-carbon monoxide flame balls and the effects of a radiation model in which self absorption is included.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/94 EXPIRATION: 4/98

PROJECT IDENTIFICATION: 962-22-05-60

NASA CONTRACT No.: NAG3-162

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Trees, D., Brown, T.M., Seshadri, K., Smooke, M.D., Balakrishnan, G., Pitz, R.W., Giovangigli, V., and Nandula, S.P., The structure of nonpremixed hydrogen-air flames. Comb. Sci. and Tech., 104, (October 1995).

Combustion of Rotating Spherical Premixed and Diffusion Flames in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Siavash H. Sohrab

Northwestern University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to improve the understanding of the influences of rotation and gravitational acceleration on combustion and flame extinction of spherical flames. This knowledge will aid the study of turbulent spray combustion such as found in diesel engines and pulse combustors.

Task Description:

A rotating porous-sphere burner will be set up for use with methane and butane in order to observe Lewis number effects. A high speed video camera will be used to observe the flame from the top and sides. Rotational velocities will be in the range of 0 to 200 rps. Stability contours will be determined for different fuel equivalence ratios, air flow rates, and rotational velocities. Both premixed and diffusion flames will be observed.

Task Significance:

Droplet spray combustion in turbulent conditions is a complex process dependent on multiple degrees of freedom and multiple interactions. The rotation of the droplets will contribute to the behavior of these flames, but is difficult to understand in a convective environment. Hence, studies in reduced gravity will help the understanding of the effects of droplet rotation. These droplet spray flames are found in oil burners and gas turbine engines.

Progress During FY 1996:

A new stream function has been found that describes the flow within a stationary spherical body of gas located at the stagnation-point of an axis-symmetric counterflow, parallel to the classical solution by Hill for a spherical vortex, describing flow within a stationary spherical body of gas located in a uniform flow. According to this new stream function, a spherical body of gas is formed by combination of two semi-spherical ring vortices, each located on one side of the stagnation plane. Also, it is shown that the new stream function could be used to present a cascade of concentric spherical flows, when each sphere within the cascade is composed of two-ring vortices. A general correspondence has been identified between flows within a spherical body of fluid in rotating counterflows on the one hand, and that within a rotating spherical body of fluid in non-rotating counterflows, on the other.

In another study, parallel to the classical solution of Hill for spherical vortex, two new stream functions have been found that describe the flow within a stationary cylindrical body of gas located either (1) within a stream moving uniformly perpendicular to the axis of cylinder, and (2) within a two-dimensional counterflow, with the axis of cylinder along the stagnation-line of the counterflow. In the latter case, it is found that a cylindrical body of gas is formed by combination of four counter-rotating line-vortices, one pair on each side of the stagnation plane. Also, it is shown that the second stream function could be used to construct a cascade of concentric cylindrical flows, when each cylinder within the cascade is composed of four circular line-vortices. It has been emphasized that experimental verification of the predicted solutions, as well as the study of the behavior of such cylindrical vortices may be best performed under micro-gravity environments.

By the application of large activation energy asymptotic method, stationary configuration of flame-fronts within an array of counter-rotating vortices has been investigated, using thermo-diffusive flame model. The calculated flame-front geometry is found to be in agreement with previous findings in the literature based on either numerical calculations using sub-grid models, or the eikonal equation. These results, among numerous other important applications, will help the understanding of flame-front behavior within gravitationally-unstable hydrodynamic fields, such as in Benard cells.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NAG3-186

RESPONSIBLE CENTER: LeRC

Diffusion Flame Structure, Shape and Extinction: Geometrical Considerations

PRINCIPAL INVESTIGATOR: Prof. Jose L. Torero

University of Maryland

CO-INVESTIGATORS:

Ezekoye, O.A.

University of Texas at Austin

Task Objective:

A diffusion flame established between opposing fuel and oxidizer streams with variable inlet orientation will be used to study the relative importance of diffusion and convection as heat and mass transfer mechanisms. Exploration of the effects of physical boundaries, radiation heat losses and buoyancy will complement this study.

Task Description:

The experimental configuration consists of two opposing porous burners through which fuel and oxidizer will be introduced. The orientation of both burners can be changed so that an angle can be created between the inlet surfaces. Development of the experimental hardware and ground based experimentation is planned for the years 1996-97. This experiment is specially suitable for parabolic flights and it is the objective to conduct the first parabolic flight campaign before the end of 1997.

An extension of the counter-flow diffusion flame analysis proposed by Linan (Acta Astronautica, 1, 1007-10039, 1974) that incorporates the effect of finite boundaries on the structure of the diffusion flame will also be attempted. The configuration to be studied initially will be that of opposing fuel and oxidizer flows.

Task Significance:

Diffusion controlled flames are common to many industrial processes and fire scenarios and are still far from being well understood. Microgravity provides an ideal environment to study the structure of diffusion flames because transport of fuel and oxidizer can be studied uncoupled from natural convection. The significant reduction of buoyancy allows the stabilization of low-momentum diffusion flames free from the effects of strain and turbulence permitting a more detailed study of the relative effects of different heat and mass transport mechanisms. Better understanding of the different parameters that affect diffusion flames will contribute to improved fire safety on spacecraft and the efficiency of many industrial processes.

Progress During FY 1996:

Experimental Work: Work on the experimental hardware started in August 1996. Work has been done on three different areas, the combustion chamber, the burner, and the diagnostic techniques. An existing small-scale hood has been conditioned to act as a combustion chamber for ground testing. The flow system and support structure have been improved to fit the requirements for this experiment. This work was done by two undergraduate students. A graduate student, J. Sutula, joined the group and has been concentrating his effort on the design and construction of the gas burner. A data acquisition and control system as well as two mass flow controllers have been purchased and are now operational. A review of particle tracking systems was initiated to guide equipment selection.

Modeling: In September the University of Texas group hired a Graduate Research Assistant, J. Borlik, to begin work on the NASA project. In line with the project goals of clarifying convective diffusive processes in stabilization zones for diffusion flames, Borlik has begun work on specifying stable regions for diffusion flame anchoring in boundary-layer-type diffusion flames. Initially, his analysis will be based on using boundary-layer-type approximations with Shvab-Zeldovich coupling functions to determine the fast chemistry flame locus. After this, the conserved scalar field will be post-processed to determine the scalar dissipation field and thus the regions of flame quenching. The map of mixture fraction and scalar dissipation will then be generalized for various fuel mixtures and oxidant approach velocities.

II. MSAD Program Tasks — Ground-based Research

Discipline: Combustion Science

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 6/96 EXPIRATION: 5/98

PROJECT IDENTIFICATION: 962-22-00

NASA CONTRACT No.: NAG3-196

RESPONSIBLE CENTER: LeRC

Interactions Between Flames on Parallel Solid Surfaces

PRINCIPAL INVESTIGATOR: Dr. David L. Urban

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of the proposed research is to study the interactions between flames which are spreading or established over parallel solid surfaces and to determine the relative importance of radiative and convective heat exchange versus the potential reduction of oxidizer due to the presence of the second fuel surface. The results from this work will be used to improve existing models of flame spread over solid surfaces and to improve our understanding of fire spread and growth for practical fuel geometries.

Task Description:

The research will be conducted under a ground-based program. Low gravity testing will be conducted at the NASA LeRC drop towers and on NASA's low-gravity research aircraft. The objective of this work will be to determine the dependence of flame spread over parallel sheets on geometric parameters such as height and width and to use this understanding to select the optimum configuration for more extensive tests. These tests will determine the dependence of spread rate for parallel surfaces on fuel thickness, separation distance, oxidizer flow direction and rate and gas phase radiation. In addition, the controlling factors in the unstable regime at close surface separations will be established. Tests will also be conducted to determine the flame structure and burning rate for flames established over parallel thick fuels with forced flow between the plates. Finally, these results will be combined with numerical/analytical results to determine the importance of radiative feedback, between interacting flames and surfaces, on flammability and spread and burning rates.

Task Significance:

The interaction between flames on solid surfaces is of considerable practical importance since in most practical heterogeneous combustion systems, the condensed phase is distributed in more than one piece and this spatial distribution can strongly affect burning and/or spread rate. From a fundamental viewpoint, the interaction between parallel surfaces offers opportunities to simplify the boundary conditions, over those for isolated surfaces, as the opposing surfaces impose a plane of symmetry between the two surfaces and if the surfaces are sufficiently large, the radiation shape factors between the surfaces and between the flame and the surfaces approach unity. This geometry also provides interesting and unique opportunities to explore the relative effects of reactant diffusion rates, radiative heat transport and conductive transport in flame spread; these transport mechanisms have been identified as critically important in microgravity.

These phenomena will be more readily studied in nonbuoyant flames as the buoyant transport will be removed, simplifying analysis and increasing the importance of conduction and radiation. In the absence of strong buoyant flows, the interaction between flames on opposing sheets extends to greater separation distances, providing greater opportunities to study the interaction via the greater spatial resolution afforded by microgravity.

These results will be significant to low gravity flame spread research in general as the parallel geometry with its plane of symmetry between the fuel surfaces is in some terms simpler than the traditional case of a single sheet in an infinite oxidizer. The results will be an extension of the existing body of knowledge concerning flame spread and burning rate over flat surfaces. The work might also have practical benefits as radiant preheating is also very significant in fire spread in building fires. Due to the significance of flame interaction in terrestrial fire safety, it is important that flame interactions be studied in low gravity to assess their importance in spacecraft fire safety.

Progress During FY 1996:

Progress for FY 1996

October

The chambers received from outside fabrication were found to have various deficiencies. They are being sent back to the outside vendor for repair.

The design for the conversion of the LSP Soot Volume Fraction breadboard system to an interferometer was reviewed and has been sent to the machine shop for review.

November

More components for the interferometer system have been ordered. The modification of the LSP optic components is underway. Analysis of the existing 2.2 second test data base is proceeding.

January

One of the chambers received from outside fabrication is now acceptable and is being prepared for use, the other chamber has been sent back for rewelding.

The components for the conversion of the LSP Soot Volume Fraction breadboard system to an interferometer have been fabricated and assembly is in process.

March

The reworked interferometer components and the repaired laser-diode controller were reassembled and tested. The overall design works well, providing adequate adjustability for use in the drop tower. Modification is needed to one component to allow optimization of the fringes.

May

To improve adjustability of the interferometer, a new design concept was developed by ADF which will significantly improve adjustability. The design has been approved and is in detailing.

An OAI summer student Mauricio Salinas began his summer internship. He will be conducting tests in the 2.2 Second Drop Tower.

June

Tests continued in the drop tower with Mauricio Salinas conducting a series of tests measuring spread rates for a variety of pressures.

The new components for the interferometer were delivered and installed. Improved positioning of the iris is now possible. The reference surface is being installed so calibration of the device can be conducted.

August

Hardware for the normal gravity calibration of the interferometer was machined and assembled. These tests will measure the temperature profile of a heated vertical flat plate will be conducted after the optical set-up is stabilized. Currently, vibrations from the room are disturbing the fringes. This problem should be solved with the use of a set of vibration dampers, which were ordered earlier this month. In addition, a target was machined for use with the interferometer which will be used in determining length scales in the flame images.

Calculations of adiabatic flame temperatures (EQLBRM) and mixture thermal conductivities (CHEMKIN-II multicomponent transport property code) are being made by Mauricio Salinas. The data file for EQLBRM was modified to include helium which is being used in as a diluent in the oxidizer. These parameters will be used to calculate de Ris' theoretical flame spread rate and compared to microgravity based interacting flame spread rates.

September

The positioning mechanism is being reworked. The difficulty is a result of the requirement to maintain the integrity of the existing LSP hardware while providing the required precise adjustability and drop tower shock hardening. Once that is completed the calibration tests will proceed.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/94 EXPIRATION: 5/98

PROJECT IDENTIFICATION: 962-22-05-52

RESPONSIBLE CENTER: LeRC

Gasless Combustion Synthesis from Elements Under Microgravity: A Study of Structure-Formation Processes

PRINCIPAL INVESTIGATOR: Prof. Arvind Varma

University of Notre Dame

CO-INVESTIGATORS:

McGinn, P.J.

University of Notre Dame

Task Objective:

The project is an analytical and experimental investigation of the mechanisms of reaction and structure formation during combustion synthesis of advanced materials from elemental reactants. Many of the processes, product compositions, and product morphology are affected by gravity, and conducting the syntheses under microgravity will elucidate the reaction mechanisms to give fuller understanding of the processes and their applications.

Task Description:

The mode of combustion synthesis under investigation is that of self-propagating high-temperature synthesis, wherein the reaction is initiated at one end of the sample and it self-propagates through the reactants in the form of a rapid combustion wave. The selected process is "gasless" synthesis, in which all reactants are elements in the solid state and no gaseous product appears during combustion.

Previous studies have shown that the reaction and structure-formation mechanisms in the gasless combustion-synthesis process involve several stages, including melting of reactants and products, spreading of the melt, droplet coalescence, diffusion and convection, buoyancy of solid particles and bubbles in the melt, nucleation of solid products, and crystal growth. The project aims to model, isolate, control, and optimize the above stages, taking advantage of the absence of the disturbing effects of gravity.

The experimental program covers several reactants (green mixtures). The simplest is a combination of aluminum (Al) and nickel (Ni) powders pressed into a pellet. These elements react to produce a mixture of nickel aluminides, Ni_3Al and NiAl . Another green mixture is that of a pressed powder of Ni, Al, titanium (Ti), and boron (B), which reacts to form a mixture of Ni_3Al and TiB_2 . Another, more complex, reactant configuration is that of nickel particles clad with aluminum.

The reactions are conducted in a combustion chamber under vacuum or an inert atmosphere (argon). The basic reaction support is a boron nitride plate with four slots in the form of a cross. Three of the ports are filled with green mixture pellets and the fourth with the igniter coil. The experimental variables include the composition and porosity of the green mixture and the initial temperature of the reaction. Interchangeable support plates can accommodate variations of the reaction configurations, such as expansion tubes. Diagnostics measure the combustion-front propagation velocity, temperature-time history of the process, pellet size and appearance, and the microstructure and phase composition of the products.

For tests in microgravity, the basic apparatus is employed, but diagnostics are simplified to only high-speed observations of the combustion process. The product compositions and metallurgical state are analyzed when recovered after the tests. The first series of microgravity syntheses are conducted in the NASA Lewis Research Center 2.2-Second Drop Tower Facility. Since reaction rates are rapid, combustion is essentially complete in one to two seconds time for pellets of the order of a centimeter diameter by a centimeter in length.

Further testing will take place in the NASA Lewis Research Center Reduced Gravity Airplane Facility (DC-9).

Task Significance:

The study is the first to use microgravity in this method of combustion synthesis in order to isolate the process stages and understand the reaction and structure-formation mechanisms. The microgravity test results provide a "benchmark" of processing conditions and product compositions and structure to guide ground-based processing on a larger scale. Many aerospace applications require such materials with tailored properties for performance at severe high-temperature or corrosive conditions. There is also a growing field of industrial and medical demands for these custom materials in engine components, filters, catalyst supports, and bone replacements.

Progress During FY 1996:

The combustion syntheses were performed with initial green mixtures of Al, Ni, Ti, and B to produce inter-metallic composite materials of Ni_3Al dispersed in a TiB_2 matrix. Normal-gravity testing indicated that there is a strong effect of buoyancy for the reactions with mixtures containing a high percentage of TiB_2 . Combustion is stable, but it proceeds at a temperature above the melting point of Ni_3Al . Hence, the solid TiB_2 can migrate in the denser molten Ni_3Al , affecting the microstructure and compositional uniformity of the composite product. Reactions in microgravity will modify this gravity-induced buoyancy effect and promote more uniform product microstructures.

For the initial microgravity testing, conducted in the NASA Lewis Research Center 2.2-Second Drop Tower, a specialized ignition control and power distribution circuit were needed to synchronize the ignition at the beginning of the microgravity drop sequence and to maximize the time period for combustion in microgravity. The circuitry was developed cooperatively by the NASA electrical engineer and the Notre Dame research associate. The ignition programming control contributed greatly to the success of the reaction tests conducted in the drop tower.

In the drop-tower microgravity tests, three reaction configurations were employed. 1) The volume-constrained reaction uses the basic configuration with three green mixtures in the cross-shaped ports on the support plate, each reacting simultaneously. 2) The controlled-quenching reaction uses a green mixture compressed into a wedge-shaped slot on a copper-block heat sink mounted on the support plate. 3) The expanded variable-porosity reaction uses a green mixture pellet inside a longer quartz cylinder mounted on the support plate for unconstrained expansion. Twenty successful drop tests were conducted over two separate weeks of testing in the drop tower. Each microgravity test was preceded or followed by a corresponding normal-gravity synthesis.

Qualitative assessments of the results were derived from high-speed video imaging. The volume-constrained reaction shows more rapid combustion wave velocities and apparently better product homogeneity in microgravity as compared to normal gravity. The controlled-quenching reaction shows differing degrees of completed reaction and more uniform particle size variation with distance from the quenched front. The variable-porosity reaction shows greater lengths of expansion and accordingly higher porosities in microgravity. All these results are as anticipated. The quantitative assessment of drop-tower tests through sectioning of the products and X-ray diffraction measurements of composition and scanning electron microscopic measurements of the microstructure was still in progress at the conclusion of the fiscal year.

The microgravity exposure in the 2.2-Second Drop Tower is sufficient for the completion of the reactions, but the investigators determined that the recovery at the end of the drop affected the final product properties. Accordingly, the test facility has been modified for 20-second airplane testing, which are to be initiated in the NASA Lewis Research DC-9 in October 1996.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 3
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/94 EXPIRATION: 1/97

PROJECT IDENTIFICATION: 962-22-05-56

NASA CONTRACT NO.: NAG3-164

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Yi, H.-C., Varma, A., Rogachev, A.S., and McGinn, P.J., Gravity-induced microstructural non-uniformities during combustion synthesis of intermetallic-ceramic composite materials. Ind. Eng. Chem. Research, vol. 35, pp. 2982-2985 (September 1996).

Studies of Wind-Aided Flame Spread Over Thin Cellulosic Fuels in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Indrek S. Wichman

Michigan State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to develop fundamental theoretical models for wind-aided flame spread over thin solid fuels in low gravity. An important aspect of this study is to develop detailed models for the combustion process in the flame anchoring region, the so-called "Triple-Flame" zone and for the fuel pyrolysis chemistry.

Task Description:

The theoretical modeling effort will explore two tracks, one fundamental, the other directly concerned with the wind-aided flame spread calculations. The fundamental part will be detailed examination of the triple flame problem near the leading edge of the spreading flame. The results of this model should provide the heat flux distribution to the supporting fuel surface. The solution techniques employed will be asymptotic and approximate methods combined with numerical methods. The second model to be examined will be wind-aided flame spread calculations. An order-of-magnitude analyses of the governing equations will be performed to identify the correct scaling of the wind-aided flame spread problem, particularly near the flame attachment point. The properly scaled equations will be solved numerically to obtain flame spread rates. The results of this study will be compared against experimental data obtained in low gravity facilities at the NASA Lewis Research Center as a part of other on-going programs.

Task Significance:

Theoretical models for the combustion process occurring at the flame anchoring point will be developed to better understand the triple flame structure. Using this basic model, numerical codes will be developed to predict wind-aided flame spread rates over thin solid fuels.

Progress During FY 1996:

A model of the triple flame that reproduces and explains many of its features was successfully developed. The most obvious is the flame shape, which is quite accurately predicted over a wide range of flows. Of deeper relevance is the fact that agreement has arisen through the use of a specific set of hypotheses and their associated simplifications: hence, it is possible to determine what is important and what is not in the generic makeup of the triple flame structure. This work has resulted in a manuscript submitted on 7/23/96 to Comb. Sci. Tech. entitled "The Structure of Quenched Triple Flames Near Cold Walls in Convective Flows" by I. S. Wichman, N. Lakkaraju and B. Ramadan.

The related problem of calculating quenching distances is currently under study. This is one part of the above work that was not fully explored. That is, in the above comparisons of theory and numerics one input parameter was needed, the quenching distance from the cold wall; once this was given--as the actual or numerically determined distance--the subsequent agreement for the flame shape between theory and numerics was excellent. In this work the use of asymptotics and numerical integrations where necessary in order to produce analytical/numerical formulae for the quenching distance. The formulae contain one or more coefficients that must be determined through the numerical solution of an elliptic boundary-value problem. The agreement between the asymptotic theory and the pure numerical results is very good, generally much better than 10%. A manuscript entitled "Attachment and Liftoff of Diffusion Flames Near Cold Walls With and Without Reactant Flow" by I. S. Wichman, Z. Pavlova, and B. Ramadan is under preparation.

A study of the influences of convection on flame attachment distances has been underway all of 1995-1996. Much of the theorizing is complete, but numerical testing is still being carried out. An abstract was sent to the ISSM-II Scaling Conference to be held in Kentucky in 1997. A detailed article will be prepared for Phys. Fluids in the near future. Investigators are B. Ramadan and I. S. Wichman.

A detailed model of flame liftoff and quenching is being carried out by B. Ramadan. This involves the numerical solution of the Navier-Stokes equations and the associated combustion equations. We have presented work at the APS Fluid Dynamics meeting in Irvine, CA (Nov., 1995) and we will present ongoing work in Nov. 1996 at this years' PAPS meeting in Syracuse, NY.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	2	MS Degrees:	2
PhD Students:	0	PhD Degrees:	0

TASK INITIATION: 3/94 **EXPIRATION:** 3/98**PROJECT IDENTIFICATION:** 962-22-05-53**NASA CONTRACT NO.:** NA63-162**RESPONSIBLE CENTER:** LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Ramadan, B. and Wichman, I.S., "A numerical study of two-dimensional laminar flames anchored by a dividing plate." Central States Section of the Combustion Institute, 1996.

Wichman, I. S., "Recent theoretical research on diffusion flames and premixed flames with significant heat losses." Sandia Labs invited presentation, May 17, 1996.

Wichman, I.S., and Ramadan, B., "Parametric dependencies of lifted and attached diffusion flames near cold walls." Central States Section of the Combustion Institute, 1996.

High-Pressure Combustion of Binary Fuel Sprays

PRINCIPAL INVESTIGATOR: Prof. Forman A. Williams

University of California, San Diego

CO-INVESTIGATORS:

Kono, M.
Sato, J.University of Tokyo, Japan
IHI, Inc., Japan

Task Objective:

The objective of the proposed research is to improve understanding of the combustion of sprays of multi-component fuels at elevated pressures, extending from normal atmospheric pressure to pressures above the critical pressure of the fuel. In particular, explanation of the role of previously observed three-stage droplet combustion behavior and microexplosion in spray combustion is sought. The extent to which buoyancy influences the phenomena that occur is to be determined.

Task Description:

The objective is to be achieved by theoretical analyses taking into account concentration profiles of fuel constituents within the liquid, instabilities, droplet interactions, and conditions for achieving the limit of superheat, along with drop-tower experiments employing 1.4 and 2.2-Second Drop Towers. Binary mixtures of heptane and hexadecane will be studied first, using fiber-supported droplets of diameters from 0.8 mm to 1.5 mm in air at pressures from 0.1 to 5 MPa. Later work is planned to involve free droplets and other fuels and possibly microgravity facilities that afford longer test times.

This program is a joint program with several investigators in Japan. The Science and Technology Agency of Japan is supporting research by Dr. Michikata Kono, Professor, Department of Aeronautics, The University of Tokyo, Tokyo, Japan, Dr. Takashi Niioka, Professor, Institute of Fluid Science, Tohoku University, Sendai, Japan, and Dr. Jun'ichi Sato, Senior Researcher, Heat and Fluid Dynamics Department, Research Institute, Ishikawajima-Harima Heavy Industries Co., Tokyo, Japan on "Combustion of a Fuel Droplet in High-Pressure Atmospheres under Microgravity Conditions" and on "Ignition of Fuel Droplets in High Pressure, High-Temperature Environments."

Task Significance:

The proposed research will improve our understanding of the mechanisms of the combustion of high pressure fuel sprays, such as those found in diesel and gas turbine engines.

Progress During FY 1996:

Fiber-supported droplets of mixtures of n-heptane and n-hexadecane, initially 1 mm in diameter, were burned in room-temperature air at pressures from 1 MPa to 6 MPa in the 2.2 Second Drop Tower. For most mixtures the total burning time was observed to achieve a minimum value at pressures well above the critical pressure of either of the pure fuels. This behavior is explained in terms of critical mixing conditions of a ternary system consisting of the two fuels and nitrogen. The importance of inert-gas dissolution in the liquid fuel near the critical point is thereby re-emphasized, and nonmonotonic dependence of dissolution on initial fuel composition is demonstrated. The results provide information that can be used to estimate high-pressure burning rates of fuel mixtures.

A series of tests were conducted in the 2.2 Second Drop Tower on the combustion of a two-droplet array of n-heptane and n-hexadecane, with 1 mm initial size droplets. The variables were the pressure (0.1 to 6.0 MPa), fuel mixture ratio (0.11 to 1.0 initial hexadecane mass fraction) and inter-droplet spacing ($L/D \sim 4$ to 10 and ∞). The results are being analyzed and another series of tests is planned for fall '96.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 12/94 EXPIRATION: 11/98

PROJECT IDENTIFICATION: 962-22-05-41

NASA CONTRACT NO.: NAG3-168

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Mikami, M., Habara, O., Kono, M., Sato, J., Dietrich, D.L., and Williams, F.A., Pressure effects in droplet combustion of miscible binary fuels. Combustion Science and Technology, (1996).

Presentations

Haggard, B., Dryer, F.L., Nayagam, V., Shaw, B.D., and Williams, F.A., "Droplet combustion experiments in spacelab." Twenty-Sixth Symposium (International) on Combustion, Naples, Italy, 1996.

Laser Diagnostics for Fundamental Microgravity Droplet Combustion Studies

PRINCIPAL INVESTIGATOR: Dr. Michael Winter

United Technologies Research Center

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This research program seeks to investigate the range of applicability of advanced diagnostics to droplet combustion under microgravity conditions while generating fundamental information relevant to other ongoing NASA programs. Using a progressive approach, advanced laser diagnostics will progress from laboratory to flight experiments. In this way, these diagnostics can be developed, while providing fundamental data on droplet transport and combustion phenomena. Through consultation with NASA personnel, and other researchers in the field of microgravity droplet transport and combustion, priorities have been established with respect to measurement parameters. The prioritized measurement parameters are:

1. Flame front position.
2. Relative gas-phase flow around droplets.
3. Droplet surface transport and internal flow.

Task Description:

An integrated diagnostic unit, capable of performing these measurements has been assembled under a previous contract. The unit consisting of NASA and TC owned equipment has been transferred or applied to the current contract. All of the major components such as lasers, detectors and data systems are currently allocated to this effort. A self-contained, miniature, nitrogen-pumped dye laser system and two-dimensional intensified CCD imaging system will form the core of the unit. A miniature Nd:YAG dye laser has been integrated in the Laser Diagnostics Droplet Combustion facility for measurement of hydroxyl radical concentrations.

The testing program is proceeding with ever more challenging environments proceeding from the laboratory, to flight based tests. The diagnostic approaches and instrumentation are being verified in a laboratory setting under Task II. Experiments with the intent of reducing the risks associated with high impact and droplet drift are being conducted on the Lear Jet, DC-9 and KC-135 aircraft, with fiber suspended, or electrodynamically levitated droplets. Initial measurements are being performed on use of PLIF measurements to describe flame front position. Gas-phase flow dynamics will be determined by velocity measurements using particle image velocimetry. Measurement of droplet surface and internal transport are also underway.

Task Significance:

One of the most fundamental distinctions in combustion is whether a flame is a premixed or non-premixed flame. Condensed-phase materials usually serve as reactants in practical combustion devices, either through direct injection of a condensed-phase fuel into a combustor or the initial presence of a condensed-phase fuel within the combustor. These fuels generally burn as non-premixed flames. Additionally, most hazardous flames are multi-phase diffusion flames as well. Many of these combustion systems involve burning liquid-phase fuels which are comprised of many individual droplets.

Basic understanding is best advanced by well-controlled experiments and simplified calculations. A great deal of attention has been paid to studying the combustion of individual droplets, which is the simplest example of non-premixed combustion. These single-droplet flames provide an idealized geometry for investigating the interaction of the physical and chemical processes involved. A significant means of simplifying droplet combustion is to approach the phenomena in a microgravity environment. A great deal of activity is ongoing in this area, including calculations, drop towers, the Droplet Combustion Experiment (DCE), and glove-box experiments aboard the space shuttle. Drop tower data have shown deviations from calculated results, suggesting that the experimental conditions may differ from the idealized assumptions used.

Optical diagnostics offer several advantages over physical probes because they permit nonintrusive multi-point measurements. Nonintrusive measurements are of particular importance for droplet combustion and transport in

microgravity environments, where physical contact would introduce an unacceptable level of perturbations. The resolution of these diagnostics can also isolate transport to length scales much smaller than the droplet diameter. These techniques can be configured to instantaneously map an entire flow field in two and three dimensions, providing either qualitative or quantitative information on the distribution of a desired scalar or vector quantity.

Progress During FY 1996:

Hardware:

An apparatus for performing laser-induced fluorescence measurements of fiber supported burning fuel droplets aboard the NASA Learjet and KC-135 and DC-9 aircraft facilities was designed and built primarily in 1993 with testing and use in 1994. The rig houses a self-contained miniature nitrogen-pumped dye laser system and two-dimensional intensified CCD and unintensified CCD imaging systems. The time code generators, two VCR s, a timing system, and MacIntosh IIfx computer with image digitization hardware form the data collection/storage system. Droplet deployment, ignition and synchronization to the timing electronics is accomplished via a unique system of radio controlled model airplane controls.

Experiments:

A new multi-level combustion platform has been fabricated and tested aboard the DC-9 which includes a levitator. This module is a direct replacement to the original and can be replaced in a matter of minutes between flight tests, or parabolas.

The design relies upon electrodynamic levitation and the electrostatic levitation electrodes are passive. While this increases the difficulties associated with 1-g testing, it significantly increase the optical access and preclude flame interferences at 0-g where the flame stand off distances are significantly greater. This system is undergoing modifications to optimize its performance based on testing during FY96.

Levitator modifications including a variable high-voltage droplet charging system should allow more versatile use in tests planned aboard the DC-9 aircraft. The charging system places up to 6000 volts directly on the deployment needle. Increasing the charge should also allow greater flexibility in ground testing the apparatus.

UTC has provided a new Nd:YAG laser from Big Sky Laser of Montana. The laser specifications are for 200 mj at 532 nm and 20 Hz. The laser has been implemented in the apparatus and is functioning properly.

A milestone of this project agreed to by Dr. Vander Wal is the acquisition of 2-D images of OH fluorescence from a burning droplet in micro-gravity. The fluorescence may be excited from radiation at several wavelengths including the 0,0 band at 308 nm and the P1(1) transition at 282 nm. For either case, the fluorescence is observed in the 308 nm band. Clearly, excitation at 282 nm is preferred because the signal can be spectrally separated from the excitation radiation. The experiment will require a few millijoules of energy at 282 nm to excite the OH molecules over a laser sheet height of 15 mm. A cost effective laser design utilizes available equipment to produce a reliable system that can operate within the constraints of the micro-gravity environment. Flight regulations impose some restrictions on the size and weight of the experimental hardware.

A dye laser has been built to produce 564 nm light that can be frequency doubled in a KDP crystal to produce light at 282.2 nm. It will utilize the Big Sky Nd:YAG laser for pump power. A commercial dye laser module from UTRC inventory has been substantially modified for this application. This module is compact and contains elements that allow tuning the output wavelength over the gain region of the dye, in this case, Rhodamine 590. The cavity is a modified Littrow configuration and has been modified to incorporate a flowing oscillator cell and an amplifier system. The output is doubled with KDP crystals. The compact Nd:YAG laser and modified dye laser module will easily fit within the hardware rack used for the previous flight experiments. Testing will commence aboard the DC-9 in early FY97.

Results:

Successful radical chemiluminescence, PLIF and visible flame luminosity images were obtained. Analysis indicates that the broadband visible flame luminosity and radical chemiluminescence agree well in mapping the flame front position. Comparison between the broadband visible flame luminosity and simultaneous PLIF images of NaCl seeded burning methanol droplets indicates that the visible luminosity is not a reliable marker of the flame front position, being dominated by Na chemiluminescence for droplets seeded with NaCl.

Images of OH PLIF have been acquired from the system at 1-g. Data acquisition in 0-g will be performed from fiber-supported and levitated droplets during FY97.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/94 EXPIRATION: 9/97

PROJECT IDENTIFICATION: 962-22-05-44

NASA CONTRACT NO.: NAS3-272

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Winter, M. "In-flight laser induced fluorescence from microgravity droplet combustion." presented at the Optical Society of America Topical Meetings Conference. Orlando, FL, March 18-22, 1996.

Winter, M., "In-flight laser diagnostics of microgravity droplet combustion." 25th International Symposium on Combustion, Poster P5-27, 1996.

Winter, M., "In-flight laser diagnostics for microgravity droplet combustion." presented at the 34th Aerospace Sciences Meeting and Exhibit. Reno, NV, Jan. 15-18, 1996.

Winter, M., "In-flight laser diagnostics of microgravity droplet combustion." poster presentation at the Gordon Conference on The Chemistry and Physics of Laser Diagnostics of Combustion, Plymouth, NH, October 1995.

Winter, M., "Laser diagnostic measurements of fundamental processes in droplets." Seminar given at Brown University, Providence, RI, October 31, 1995.

Combustion of a Polymer (PMMA) Sphere in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Jiann C. Yang

National Institute of Standards and Technology

CO-INVESTIGATORS:

Hamins, A.

National Institute of Standards and Technology (NIST)

Task Objective:

The main research objective is to determine the burning rate constants of PMMA spheres under conditions of reduced gravity, various ambient oxygen concentrations, and total pressures. The dependence of the burning rate constant on sphere size will also be explored. The results will be compared to those obtained under earth normal gravity.

Task Description:

Experiments at elevated oxygen concentrations and reduced pressures will be performed in the NASA low-gravity aircraft. This will require construction of an experimental package. The package consists of a pressure chamber, a rack to house the experimental components, a retracting mechanism to move an opposing pair of miniature Bunsen burners for ignition, a fuel (butane) reservoir, DC power supplies, an electronic spark system, a vacuum pump, a data acquisition and control system, two CCD cameras, sample holder, and a lab-top computer. The package can be used for reduced gravity experiments aboard the DC-9 or 1G experiments in the laboratory.

Task Significance:

Because of the simple sample geometry (a sphere) and reduced gravity conditions, the effect of condensed phase bubbling behavior on the burning processes can be adequately assessed without complications arising from a complex sample geometry and buoyancy-induced flow. The experimental results thus obtained will be used to test thermoplastic polymer combustion models which are needed to better understand the formation and growth of bubbles in new formulations of fire-retarded polymers.

Progress During FY 1996:

The experimental package for the NASA DC-9 Reduced Gravity Aircraft was completed in early November 1995. A safety document for the flight experiments was prepared that included the experimental procedure, a hazard analysis, an electrical and mechanical analysis, and detailed schematic drawings showing the connections among various components.

Before the low gravity flight experiments, the experimental procedure and package were tested and modified using 1G experiments. Experiments investigated the duration of the igniter flames to achieve ignition of the spheres (three different diameters, 3.18 mm, 4.76 mm, and 6.35 mm) under different oxygen concentrations (30 %, 25 %, 21 %, and 19 %) and total pressure (from 0.152 MPa down to conditions where the igniter flame could not be sustained) and optimization of the time to retract the burners away from the burning spheres.

Four flight experiments were conducted in June 1996. Some technical problems were encountered in the first three flights. During the first flight, the igniter flames could not be established. The failure was attributed to the oxygen concentration of the "zero" air cylinder because the igniter flames were established when cabin air was used. During the second and third flights, two-phase flow problems associated with the use of liquified butane caused the igniter flames to persist even after the fuel flow was terminated. The igniter flames interfered with the burning spheres. The butane flow problem was corrected subsequently, by flowing the ullage vapor from the fuel reservoir instead of relying on the flashing of the liquified butane in the tubing connected to the burners. The fourth flight experiments were successful as all fifteen samples carried aboard were burnt and their burning histories and temporal variation of the temperature at the center of the suspended spheres were recorded. The experimental conditions investigated on that flight were: (1) spheres with the three different diameters, (2) 25 % ambient oxygen, (3) total pressure of 0.101 MPa, and (4) suspended thermocouples with diameters of 75 and 125 microns.

In addition to the flight experiments, a series of 1G experiments have been conducted. The 1G tests performed so far explored the following conditions: (1) three diameters, (2) two oxygen concentrations (21 % and 25 %), and (3) total pressures of 0.101 MPa, 0.083 MPa, 0.069 MPa, and 0.062 MPa.

For the 1G experiments, the temperature was observed to continue to rise until the melting sphere detached from the suspended thermocouple. A sharp rise in the temperature trace was recorded as the thermocouple junction traversed the flame. The rate of temperature increase (dT/dt) is dependent on the size of the sphere; the rate is slower for larger spheres.

For low G experiments, the reduced gravity period provided by the DC-9 aircraft is still not long enough to obtain complete burning histories for spheres with initial diameters greater than 3 mm. The average burning rate constant (obtained from the slope of the square of the diameter versus time plots) from the data obtained using 3.18 mm spheres is 1.6 mm²/s at 0.101 MPa and a 25 % ambient oxygen concentration. Extinction was not observed. The diameter measurements were obtained from the video records using a frame grabber and image analysis software. However, the extraction of burning rate constants from spheres with diameters greater than 3 mm was not possible because the diameters of the bubbling spheres did not appear to change significantly (except for some initial swelling) during the reduced gravity period. The dT/dt curves showed similar trends at low G, i.e., the rate of temperature rise was observed to be faster for smaller spheres. An anomaly in the temperature trace was found in all the 3.18 mm sphere experiments in that a period of constant temperature was present after an initial continuous temperature rise. This artifact was caused by displacement of the thermocouple junction to the exterior of the burning sphere as the polymer melted.

Examination of the video record shows that ejection of molten material into the gas phase happens more frequently in reduced gravity than in 1G. In low gravity, the ejection is more violent and frequent for the 3.18 mm spheres as compared to the 4.76 mm and 6.35 mm spheres burning in low gravity.

STUDENTS FUNDED UNDER RESEARCH:**TASK INITIATION: 5/94 EXPIRATION: 4/98****PROJECT IDENTIFICATION: 962-22-05-63****NASA CONTRACT NO.: C-32017-C****RESPONSIBLE CENTER: LeRC**

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Yang, J.C., Hamins, A., Gorchkov, N., and Glover, M., "Combustion of polymethylmethacrylate spheres." 26th International Symposium on Combustion 1996.

Yang, J.C., Hamins, A., Gorchkov, N., and Glover, M., "Combustion of polymethylmethacrylate spheres at normal and reduced gravity." Annual Conference on Fire Research, October 28-31, 1996.

Study of Two-Phase Flow and Heat Transfer in Reduced Gravities

PRINCIPAL INVESTIGATOR: Dr. Davood Abdollahian

S. Levy, Inc.

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective is to conduct two-phase flow instability studies in vertical upflow and downflow, in both a normal gravity environment and in low gravity aboard an aircraft, to ascertain the effect of gravity on instability and boiling mechanisms.

Task Description:

The approach is to design and build a recirculating flow boiling loop which would be used aboard an aircraft to test different two-phase flow instability phenomena and measure the conditions at which critical heat flux occurs. Specifically, the instability phenomena to be examined are the following: nucleation instability, flow pattern instability, excursive instability, oscillatory instability, and density wave instability. Testing would consist of examining the flow stability and critical heat flux in normal-gravity vertical upflow and downflow as well as in low gravity aboard an aircraft.

Task Significance:

Two-phase instabilities have been responsible for a multitude of fatal and costly accidents on Earth in the oil, electric power and nuclear industries. In addition, by understanding critical heat flux better, it may be possible to improve the cooling of microcircuitry used in the electronic industry thus improving the capability of that circuitry.

Progress During FY 1996:

The flow loop and instrumentation were fully integrated onto the DC-9 aircraft and several tests were conducted. There were several problems encountered with the operation of the flow loop that either corrected or fixes were identified. The first problem involved the cooling water flow loop and ice bath expelling water into the cabin. The flow loop was originally designed to dump water directly into a ice chest and then draw its supply from that chest. The flow loop was replumbed to pass the water through a copper tube which was immersed in the ice chest. System temperature and pressure conditions are set via the pre-heater and heater controllers. Because of difficulties with the operator workload, it was decided to use for future flights, an automated temperature controller.

The automatic temperature controller was used to prevent wall burnout by shutting power off to the heater and flooding the test section with cool test fluid, and this controller is connected to a thermocouple mounted to the top surface of the flow channel. For the critical heat flux (CHF) testing, care had to be exercised in turning on and off heater power since during the 2 g portion of the trajectory, the top surface would dry out and the temperature would rapidly rise increasing the potential for the automatic temperature controller to react.

During the critical heat flux tests, it was determined that there was a significant increase in the system pressure during the transition from high gravity to low gravity during the parabola. It was surmised that the increase in the pressure was due to the fact that the top of the test section had dried out in the high g portion of the trajectory and was rewetted during the low gravity period resulting in an significant increase in the vapor generation rate.

A limited number of parallel channel instability tests were conducted and the preliminary results indicate that for those test conditions, the system performed in a stable manner.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	1
MS Students:	1	MS Degrees:	1
PhD Students:	0	PhD Degrees:	0

TASK INITIATION: 3/93 EXPIRATION: 3/96

PROJECT IDENTIFICATION: 962-24-05-50

NASA CONTRACT NO.: NAS3-265

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceeding

Abdollahian, D., Quintel, J., Zahm, J., and McQuillen, J., Experimental and Analytical Study of Two-Phase Flow Parameters in microgravity. NASA Conference Publication, 3338, pp. 103-108 (1996).

Experimental and Analytical Study of Two-Phase Flow Parameters in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Davood Abdollahian

S. Levy, Inc.

CO-INVESTIGATORS:

Barez, F.
Quintal, J.San Jose State University
S. Levy, Inc.

Task Objective:

The objectives are to conduct series of tests to ascertain the effect of normal gravity in both vertical upflow and downflow conditions and reduced gravity on the hydrodynamic instability, critical heat flux and two phase pressure drop; and develop mechanistically based models for the critical heat flux and pressure drop.

Task Description:

The approach is to modify an existing rig, which was designed and built under NASA Contract NAS3-26550, to accommodate other, more environmentally-friendly, refrigerants and to account for the operational and logistical difficulties encountered during the reduced gravity testing under the prior contract. The changes that will be made include changing the orientation of the test section from a horizontal to a vertical mounting, incorporating an automatic temperature controller that would drive the preheater, and rewiring the package to facilitate easier integration into the DC-9 aircraft. Testing would consist of examining the flow stability and critical heat flux in normal-gravity vertical upflow and downflow as well as in low gravity aboard an aircraft.

Task Significance:

Two-phase instabilities have been responsible for a multitude of fatal and costly accidents on Earth in the oil, electric power and nuclear industries. In addition, by understanding critical heat flux better, it may be possible to improve the cooling of microcircuitry used in the electronic industry thus improving the capability of that circuitry.

Progress During FY 1996:

The flow loop and instrumentation were rewired at NASA LeRC and shipped back to the principal investigator. The principal investigator is researching suitable replacement refrigerants that can be utilized within the rig that will satisfy the necessary requirements for compatibility with the existing flow loop and safety related issues.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAS3-960

RESPONSIBLE CENTER: LeRC

Colloids & Nucleation

PRINCIPAL INVESTIGATOR: Prof. Bruce J. Ackerson

Oklahoma State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Direct observations will be made of the nucleation and early growth of crystals comprised of polymethylmethacrylate (PMMA) "hard" colloidal spheres in an index matching solvent. Colloidal samples will be prepared in a particle volume fraction range which exhibits crystals of colloidal particles at equilibrium. These samples will be shear melted and the subsequent appearance of crystals monitored by direct observations/video camera recording at the first order Bragg scattering angle.

Task Description:

1. Apply classical nucleation theory in the limit applicable to hard sphere interactions to compare against data. Modern analytic (density functional) and simulation results will be compared with data as appropriate.
2. Establish the practical limiting density supersaturation that can be studied without interference due to sedimentation induced convection.

Task Significance:

The experimental observations of nucleation and early growth of crystals comprised of "hard" colloidal spheres will provide a critical test of classical nucleation theory.

Progress During FY 1996:

Following an attempt to measure nucleation and crystal growth in 430nm radius PMMA particle suspensions, where the crystals proved to be too small for measurement, we recovered and cleaned a small amount of 220nm radius PMMA particle samples, made a series of volume fractions and determined the volume fraction from the measured phase diagram. The sample volume fractions were in the liquid-crystal coexistence region. Samples were "shear melted" and recrystallization was monitored at the first order Bragg scattering angle for visible light. Both crystals oriented to Bragg scatter light (which appear brightly colored) and crystals oriented in other directions (which appear dark) are visible. The crystal size and number were monitored as a function of time. The nucleation rate density was estimated from these measurements and compared well with the nucleation rate densities measured by small angle light scattering and Bragg angle scattering on similar samples where the measurement volume fractions overlap (near 0.52). However, these estimates are about three orders of magnitude less than that predicted by classical nucleation theory. For volume fractions approaching the freezing value (0.494), the nucleation rate density exhibits a much weaker dependence on volume fraction than observed near 0.52. The volume fraction dependence of classical nucleation theory is much more pronounced and similar to that observed near 0.52. This is not understood, especially since the classical theory is expected to work best near the freezing point.

Near the freezing point the crystallites formed are smaller than expected from extrapolation of small angle light scattering and other direct observations results. The low crystal density in samples near the freezing point allows more rapid settling of the crystals. The resulting larger crystal surface shear stresses may inhibit growth or the transit time across the cell restricts the growth time.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 1
PhD Students: 0

TASK INITIATION: 6/94 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-24-05-78

NASA CONTRACT NO.: NAG3-162

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Davis, K.A., Acton, S.T. and Ackerson, B.J., "Segmentation of colloidal crystal images by local histogram analysis." Proceedings of the 1996 Southwest Symposium on Image Analysis and Interpretation Proceedings, pages 178-183, 1996.

Presentations

Ackerson, B.J., He, Y. and Davis, K., "Growth and morphology of crystals made of hard spheres." NASA Fluid Physics Conference, NASA Lewis, Cleveland, Ohio, June, 1996.

Davis, K.A., Acton, S.T. and Ackerson, B.J., "Segmentation of colloidal crystal images by local histogram analysis." IEEE Southwest Symposium on Image Analysis and Interpretation, San Antonio, Texas, April, 1996.

Study of Nonaxisymmetric Liquid Bridges

PRINCIPAL INVESTIGATOR: Prof. J. Iwan D. Alexander

University of Alabama, Huntsville

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Theoretical and experimental investigation of the stability of axisymmetric and nonaxisymmetric bridges contained between equal and unequal radii disks as a function of Bond and Weber number with emphasis on the transition from unstable axisymmetric to stable nonaxisymmetric shapes.

Numerical analysis of the stability of nonaxisymmetric bridges between unequal disks for various orientations of the gravity vector.

Experimental and theoretical investigation of large (nonaxisymmetric) oscillations and breaking of liquid bridges.

Task Description:

This project involves both experimental and theoretical work. Static and dynamic experiments are conducted in a Plateau tank which makes a range of static Bond numbers accessible. Theoretical investigation includes both analytical and numerical approaches.

Task Significance:

A liquid bridge, or captive drop, is a mass of liquid held by surface tension between two or more solid supports. Liquid bridges occur in a variety of physical and technological situations and a great deal of theoretical and experimental work has been done to determine axisymmetric equilibria for various disk configurations, bridge aspect ratios and rotations. There have also been numerous investigations of the dynamics of axisymmetric liquid bridges subject to different excitations (impulses, vibration, etc.). Such investigations have been motivated both by practical considerations and basic scientific interest. Liquid bridges and drops are important factors when considering propellant management in liquid fuel chambers and in the positioning of liquid masses using surface tension forces. In crystal growth, they are associated with the floating-zone growth technique. Their oscillation and relaxation properties can also be used for viscosity and surface tension measurements of molten materials at high temperatures. Pendular liquid bridges occur widely in the powder technology industry and are a major influence on powder flow process and mechanical properties. In porous media flow, liquid-liquid displacement can lead to evolution of pendant and sessile lobes or lenticular bridges. The formation of liquid bridges from the gel that coats lung micro-airways results in occlusion of the bronchioles and is a precursor to respiratory problems and lung collapse. In addition, liquid bridges have been involved in a number of past microgravity and our research will provide results useful for the quantitative assessment of g-jitter effects on such experiments.

Progress During FY 1996:

This is a new project which just started in July, 1996. The minimum volume stability analysis is being extended to include an investigation of maximum volume limits for the effects of nonaxial acceleration on liquid bridges.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-186

RESPONSIBLE CENTER: LeRC

Stability Limits and Dynamics of Nonaxisymmetric Liquid Bridges

PRINCIPAL INVESTIGATOR: Prof. J. Iwan D. Alexander

University of Alabama, Huntsville

CO-INVESTIGATORS:

Perales, J.M.

Universidad Politecnica de Madrid

Meseguer, J.

Universidad Politecnica de Madrid

Task Objective:

Theoretical and experimental investigation of the stability of axisymmetric and axisymmetric bridges contained between equal and unequal radii disks as a function of Bond and Weber number with emphasis on the transition from unstable axisymmetric to stable nonaxisymmetric shapes.

Numerical analysis of the stability of nonaxisymmetric bridges between unequal disks for various orientations of the gravity vector.

Experimental and theoretical investigation of large (nonaxisymmetric) oscillations and breaking of liquid bridges.

Task Description:

This project involves both experimental and theoretical work. Static and dynamic experiments are conducted in a Plateau tank which makes a range of static Bond numbers accessible. Theoretical investigation includes both analytical and numerical approaches.

Task Significance:

A liquid bridge, or captive drop, is a mass of liquid held by surface tension between two or more solid supports. Liquid bridges occur in a variety of physical and technological situations and a great deal of theoretical and experimental work has been done to determine axisymmetric equilibria for various disk configurations, bridge aspect ratios and rotations. There have also been numerous investigations of the dynamics of axisymmetric liquid bridges subject to different excitations (impulses, vibration, etc.). Such investigations have been motivated both by practical considerations and basic scientific interest. Liquid bridges and drops are important factors when considering propellant management in liquid fuel chambers and in the positioning of liquid masses using surface tension forces. In crystal growth, they are associated with the floating-zone growth technique. Their oscillation and relaxation properties can also be used for viscosity and surface tension measurements of molten materials at high temperatures. Pendular liquid bridges occur widely in the powder technology industry and are a major influence on powder flow process and mechanical properties. In porous media flow, liquid-liquid displacement can lead to evolution of pendant and sessile lobes or lenticular bridges. The formation of liquid bridges from the gel that coats lung micro-airways results in occlusion of the bronchioles and is a precursor to respiratory problems and lung collapse. In addition, liquid bridges have been involved in a number of past microgravity experiments and our research will provide results useful for the quantitative assessment of g-jitter effects on such experiments.

Progress During FY 1996:

Our research involves an experimental and theoretical investigation of the statics and dynamics of nonaxisymmetric bridge configurations and nonaxisymmetric oscillations of initially axisymmetric bridges. During FY96, the effects of nonaxial acceleration on the minimum volume stability limit have been studied numerically. The minimum volume stability limit was found to be substantially modified as the lateral component of acceleration is increased. It appears to approach, but not meet, the "zero Bond number" minimum volume limit for purely axial acceleration. This analysis has since been extended to include an investigation of maximum volume limits.

We also investigated equilibrium stability problems for multiparametric axisymmetric equilibrium states. The stability of a bridge subject to the combined effect of an axial gravity and isorotation is considered when restrictions typical for the floating zone technique are accounted for. The influence of unequal disk radii combined with an axial gravity on the entire boundary of stability with respect to arbitrary perturbations is also analyzed. We also undertook theoretical and experimental investigations on the behavior of the weightless bridge when its axisymmetric shape loses stability.

For coaxial disk supports, the stability of nonaxisymmetric bridges subject to axial gravity has also been investigated experimentally and through numerical simulation. This is the first attempt that we are aware of to determine the stability limit of nonaxisymmetric bridges for ranges of relative volume and aspect ratio beyond the maximum volume margin for axisymmetric bridges.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 12/92 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 552-24-05-60

NASA CONTRACT NO.: NAG3-138

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Alexander, J.I.D., Zhang, Y., Delafontaine, S., and Fedoseyev, A., Numerical simulation of liquid bridge dynamics and statics. *Iz. Mekanika i gaza*, (1996).

Lyubimov, D., Lyubimov, T., Alexander, J.I.D., and Lobov, N.I., On the Boussinesq approximation for fluid systems with deformable boundaries. *Journal of Fluid Mechanics*, (1996).

Slobozhanin, L., Alexander, J.I.D. and Resnick, A., Bifurcation of the equilibrium states of a weightless liquid bridge. *Physics of Fluids*, (1996).

Proceedings

Alexander, J.I.D., Delafontaine, S., Resnick, A., and Zhang, Y., "Large deformations of liquid bridges." *Proceedings of the 2nd Symposium on Fluids in Space*, Naples, Italy, April 22-26, 1996.

Slobozhanin, L., Alexander, J.I.D., and Resnick, A., "Stability of Liquid bridges under reduced gravity." *Proceedings of the 2nd Symposium on Fluids in Space*, Naples, Italy, April 22-26, 1996.

Presentations

Alexander, J.I.D., "Large deformations of liquid bridges." Invited presentation at The Second Symposium on Fluids in Space, Naples, Italy, April 22-26, 1996.

Investigations of Multiple-Layer Convection

PRINCIPAL INVESTIGATOR: Prof. C. D. Andereck

Ohio State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The convection patterns that develop in two-layer fluid systems are to be studied. The principal objectives are:

1. To test the predictions of theoretical investigations.
2. To study the interaction of the pattern in one layer with the pattern in the other layer.
3. To determine the role of the geometry of the test cell on the patterns that emerge.
4. To determine the impact of surfactants at the fluid interface on the interface profile and the patterns that form.

Task Description:

An experimental investigation of natural, buoyancy driven, convection in a system consisting of two superposed layers of immiscible fluids will be performed. Narrow, pseudo-one-dimensional, test cells will be constructed with insulating side walls and conducting top and bottom walls. Temperature control of the horizontal surfaces will be provided initially by circulating known temperature water next to these surfaces. Shadowgraph visualization techniques, which are sensitive to index of refraction variations resulting from temperature gradients in the fluids, will be used to determine the flow patterns. This allows for observations of the basic dynamics of competing instabilities in the two layers. A direct comparison will then be possible between existing general theories of pattern competition, and experimental results for a specific system. This will also provide a test for direct numerical simulations of two fluid layer systems. Further work to be performed includes studying the deformation of the interface as a function of control parameter and with the introduction of surfactants. Finally, the geometry of the cell will be varied. To introduce periodic boundary conditions in one dimension we will construct an annular cell. Another variation will be to construct a cell with large extent in both horizontal dimensions, thereby freeing the system to choose more complex competing patterns.

Task Significance:

Multiple-layer convection is of interest in geophysical, astrophysical and industrial settings. It is also of importance as a fundamental pattern forming nonequilibrium system. These experiments will provide a quantitative test of our theoretical understanding of this fluid dynamical system. Results on the pattern formation processes may also be directly relevant, in thin layer limits, to understanding and improving film coating processes.

Progress During FY 1996:

We have constructed and used two basic test cells, and have employed shadowgraph and Schlieren imaging to view the convection patterns. The first cell is rectangular and consists of glass sidewalls and aluminum blocks on the top and bottom. The dimensions are such as to impose a strong alignment of convection rolls with their axes parallel to the optical path. During initial runs, the top and bottom blocks were cooled and heated, respectively, by water from temperature controlled circulators. Recently we have replaced the circulating water through the bottom block with a resistive heater and computer controlled feedback for control. With this cell we have explored the behavior of Rhodorsil 47v10 silicone oil over Fluorinert FC-70. For experiments with Rhodorsil 47v2 over water we replaced the glass sidewalls with Plexiglas walls with a minute horizontal groove machined all the way around the cell to pin the interface between the two liquids. The optical system consists of a high-intensity red LED, a large collimating lens to produce approximately parallel light entering perpendicular to the side of the cell, a focusing lens, a knife edge in the case of Schlieren, and a CCD video camera with a PC-based image capture and processing system. During this year we have also constructed a second distinct experimental system, this one in the form of an annulus. The inner and outer rings are of Plexiglas, and the top and bottom surfaces are again of aluminum. This gives us an approximately 1-D system of rolls, their axes oriented radially from the center of the annulus, with no

end walls to influence the behavior. This also gives us many more roll pairs compared with the rectangular system, thus more effectively approaching the infinite system limit. To observe the patterns in this case requires the use of a shadowgraph technique, but with a rather different optical path than for the rectangular cell. In this case the collimated light hits a conical mirror placed at the center of the annulus. The light is reflected from this mirror radially outward through the annulus, where it hits a cylindrical mirror and reflects back radially through the cell. It now hits the conical mirror, reflects off a beam splitter and goes to the CCD camera. We have now succeeded in producing shadowgraph images that cover the entire annulus with the exception of four regions covered by small bolts that hold the apparatus together. In the future this will be redesigned to eliminate these blockages.

The procedure followed in data collection is to first establish a desired depth ratio for the two fluids, and then allow the system to equilibrate for at least 12 hours at zero temperature difference between the top and bottom plates. The temperature is then ramped very slowly (effective rate of about 0.2 C per day) and data are gathered after each increment, with a suitable wait to reach a steady state. Time dependence in the Silicone oil/Fluorinert system, when it occurs, has a period on the order of one hour, so a data run consists of acquiring a single video line in each layer every 30 seconds over a total period of 6 to 8 hours. (The Silicone oil/water oscillations are faster, so somewhat less time is needed in that case.) The frames are then put together to produce space-time plots, and power spectra in space and in time are computed to obtain pattern wavelengths and frequencies.

One of the important objectives of our experiment was to explore the interaction of the pattern in one layer with the pattern in the other. In particular, numerous theoretical studies predicted oscillatory states should exist. To our knowledge, no previous experiment had shown this behavior. These oscillatory states consist of an alternation between thermal and mechanical coupling between the roll patterns. The thermal case consists of the alignment of hot rising fluid in both layers, causing rolls that are aligned one above the other to turn in the same direction, either clockwise or counterclockwise. Mechanical coupling is the alignment of the cold falling fluid in one layer, say the lower, with the hot rising fluid in the upper layer, with the result being that the rolls turn in opposite directions in a gear-like fashion. Theoretical studies have shown that, in general, stationary thermal coupling should occur for thin lower layers, while stationary mechanical coupling should occur for thick lower layers. In between, the two modes interact so as to produce an oscillatory pattern. We carried out a systematic study of this prediction by varying the depth ratio for our two different pairs of fluids, aided by weakly nonlinear stability studies carried out by Y. Renardy.

Our principal results are as follows. For the Silicone oil/Fluorinert system we have found stationary mechanical coupling for Fluorinert depths down to 36% of the total cell height, and stationary thermal coupling for smaller depths. In the range of Fluorinert depths between 36% and about 39% of the total depth we have found oscillatory states just above the onset of the stationary mechanically coupled pattern, states which persist to at least twice the critical temperature difference from the bottom to the top of the system. Both standing and traveling wave states exist, depending on the depth ratio. These results have been largely confirmed in the annular system. In addition, the wavelengths and frequencies are rather close to the theoretically predicted values for our fluids. In the annulus we typically find several dislocations as well, sources or sinks for rolls that prevent the pattern from simply rotating around the cell. For the Silicone oil/water system we have examined only three depth ratios since the necessity for a groove in the sidewalls makes it difficult to change depths. In those three cases, for water depths of 0.6, 0.67, 0.71, the pattern at onset is oscillatory, the first known realization of this behavior in a two-layer convection system. The behavior is chaotic in appearance, but the details of this behavior have not yet been documented.

We are now completing our survey of the states possible in both sets of fluids. It will be particularly important to examine the behavior of the Silicone oil/water system in the annulus, where the lack of end walls may lead to a simplified behavior at onset. In the future it will be extremely interesting to examine the patterns in a wide system where the rolls are not strongly pinned to one orientation. Predictions exist for a wide variety of possible behaviors under those conditions.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 6/94 EXPIRATION: 2/97

PROJECT IDENTIFICATION: 962-24-05-79

NASA CONTRACT NO.: NAG3-161

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Colovas, P.W., Degen, M.M., and Andereck, C.D., Observations of time-dependent behavior in a two-layer Bernard System of rectangular geometry. Bull. Amer. Phys. Soc., vol. 40, (October 1995).

Degen, M.M., Colovas, P.W., and Andereck, C.D., Convective flow in two immiscible fluid layers in an annular geometry. Bull. Amer. Phys. Soc., vol. 40, 1955 (October 1996).

Proceedings

Andereck, D.C., Colovas, P.W., and Degen, M.M., "Observations of time-dependent behavior in the two-layer Rayleigh-Bénard system." Proceedings of the workshop "Analysis of multi-fluid flows and interfacial instabilities," 1996.

Andereck, D.C., Colovas, P.W., Degen, M.M., "Observations of time-dependent behavior in the two-layer Rayleigh-Benard system." Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, Ohio, June 13-15, 1996.

Presentations

Andereck, D.C., "Instabilities in multiple-layer convection." Society of Engineering Science Annual Meeting, Chandrasekhar Memorial Symposium, Tempe, Arizona, October 1996.

Electrokinetic Transport of Heterogeneous Particles in Suspensions

PRINCIPAL INVESTIGATOR: Prof. John L. Anderson

Carnegie Mellon University

CO-INVESTIGATORS:

Garoff, S.

Carnegie Mellon University

Task Objective:

There were two objectives to our research program. The first was to develop a hydrodynamic theory for the rotation of heterogeneous colloidal doublets in electric fields. The second objective was to design and use an experimental system to measure the tangential and normal forces between colloidal particles using electrophoresis. In the course of this work we developed the method of "differential electrophoresis."

Task Description:

1. If a colloidal doublet is formed by coagulating two particles with different zeta potentials (i.e., surface charge densities), the resulting aggregate, called a "heterogeneous doublet," has a dipole moment. Due to this dipole moment, heterogeneous doublets rotate in applied electric fields at a rate proportional to the difference in zeta potentials on the two moieties. Using a hydrodynamic theory based on the Lorentz reciprocal theorem for Stokes flow, we have obtained the rotation rate of the doublet in terms of explicit algebraic expressions; heretofore, the rotation rate was determined by numerically solving the electrohydrodynamic equations. Since the rotation rate of a doublet reveals the state of adhesion between the two particles (i.e., whether the particles rotate in tandem or whether their surfaces slip past each other), this theory is essential for interpreting our experimental data for doublet rotation rates in terms of the tangential forces acting between the surfaces of colloidal particles.
2. After a heterogeneous doublet rotates into alignment with an applied electric field, the two particles in the doublet tend to pull apart. By examining the rotation rate and the electric field at which the doublet finally breaks into two particles, we can determine the limits of the tangential and normal colloidal forces between the particles. Data has been collected at a variety of solution conditions (pH, ionic strength) for polystyrene latex particles of different surface chemistry. The measured forces are more than 50 times greater than those predicted by the conventional DLVO theory for colloidal forces. This work will continue for mineral colloids (e.g., silica particles).

Task Significance:

To engineer the processing of suspensions of colloidal particles (e.g., paint, glue, crushed mineral ore, paper pulp), one must understand the suspension properties. This ultimately requires a knowledge of the forces between colloidal particles. Our experimental and theoretical program aims to determine these forces under a variety of conditions. The current theoretical model for these forces, DLVO theory, has many shortcomings and has failed to explain many experiments involving both polymeric and mineral particles. Our experiments aim to highlight conditions for which the DLVO theory fails or succeeds and to provide data by which to compare future theories.

One limitation in pushing the technique of differential electrophoresis to more general colloidal species than just latex (specific gravity 1.05), for example minerals (specific gravity > 2.0), is the confounding effect of gravity. Micron-size particles with these higher densities will orient and settle because of the earth's gravitational field, thus clouding interpretation of the measured kinematic response of the colloidal doublets and other shaped particles.

Progress During FY 1996:

The "differential electrophoresis" technique was developed to probe the forces holding a colloidal doublet together. The colloids were polystyrene latex spheres having various surface groups to impart a charge. Differential electrophoresis takes advantage of the difference in zeta potential of two particles in a doublet to study the lateral and normal forces between the particles. By measuring the rotation rate of the doublet we were able to determine the extent of rigidity of the doublet; rigid-body rotation of the doublet means the surfaces of the particles cannot move relative to each other. When the doublet aligned with the electric field then the electrophoretic force tending to separate the particles was increased by increasing the electric field; this is called "electrophoretic displacement."

Our experimental results for electrophoretic rotation and displacement of latex doublets indicated rigid-body rotation in all cases, and the displacement studies failed to break any doublets even when forces as great as 50 pico newtons were applied. These results are inconsistent with the classical theory (DLVO) of colloidal forces, which predict a secondary minimum between the latex particles in a doublet under the conditions of our experiment. Our conclusion based on the experimental results is that the DLVO theory is in serious error for the latex particles of our experiment. This experimental work has been published by D. Velegol and J.L. Anderson in the technical journal *Langmuir* (vol. 12, p 4103, 1996 - "Determining the Forces between Polystyrene Latex Spheres Using Differential Electrophoresis"). We have developed a mathematical analysis for conduction processes in the thin gap between two spheres. The analysis allows for a nonuniform conductivity in the gap and a uniform conductivity outside the gap. This work has been submitted for publication.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 1/93 **EXPIRATION:** 1/96

PROJECT IDENTIFICATION: 962-24-08-09

NASA CONTRACT NO.: NAG8-964

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Anderson, J.L. Electrokinetic Transport of Colloidal Particles with Heterogeneous Surfaces. *J. Electrostatics*, vol. 34, 189 (1995).

Solomentsev, Y., and Anderson, J.L. Electrophoretic Transport of Spheroidal Colloids in Nonhomogeneous Electric Fields. *I&EC Research*, vol. 34, 3231 (1995).

Velegol, D., and Anderson, J.L. Probing the Structure of Colloidal Doublets by Electrophoretic Rotation. *Langmuir*, vol. 12, 675 (1996).

Velegol, D., and Anderson, J.L. Determining the Forces between Polystyrene Latex Spheres Using Differential Electrophoresis. *Langmuir*, vol. 12, 4103 (1996).

Experimental Study of Liquid Jet Impingement in Microgravity: The Hydraulic Jump

PRINCIPAL INVESTIGATOR: Prof. C. T. Avedisian

Cornell University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This study was initiated to improve the understanding of the effect of gravity on a circular hydraulic jump (CHJ) formed from a laminar circular jet. To isolate the influence of gravity, the fluid and target surface temperatures were the same. Specific objectives were to 1) determine the extent to which a CHJ could be stabilized within the allotted experimental time, 2) measure the evolution of a CHJ upon a sudden transition from normal gravity (i.e., $G/g_0=1$ where $g_0=9.8\text{m/s}^2$) to microgravity ($G\ll 1$), and 3) compare the results with available analyses to predict the CHJ diameter. The primary parameter in the experiments was the fluid level downstream of the jump and the liquid flow rate. Water was the working fluid. Information gained from this preliminary effort will be important for designing an experiment to study heat transfer due to an impinging jet onto a hot surface in microgravity, which will require significantly longer times for observation and data acquisition than were available to the effort described here. This research is considered to be a preliminary effort to studying heat transfer from impinging jets in microgravity. It was budgeted as a one year feasibility study, and was completed this past year under a no-cost extension.

Task Description:

A prominent feature of an impinging liquid jet is the potential for formation of a hydraulic jump, which is the sudden increase in fluid film thickness and associated decrease in film velocity that sometimes occurs when a radial jet impinges onto a surface. Gravity influences two aspects in this process: 1) the position of the jump, and 2) the shape of the jump profile. The primary task of this research was to design an experiment to view the evolution of a CHJ upon a transition from $G=1$ to $G\ll 1$, to allow for control of the downstream height and liquid flow rate, and to make quantitative measurements of the jump position and fluid film shape across the jump.

Task Significance:

Liquid jet impingement is an efficient means for heat transfer owing to the high heat transfer rates that are possible because of the high fluid velocities across relatively thin films that characterize the jet impingement and spreading process. However, the potential for a CHJ creates the possibility for significant degradation in heat transfer because of the reduced fluid velocity downstream of the jump compared to upstream of it. The target surface to be cooled must, therefore, be smaller than the CHJ radius. Parameters known to influence the jump location are the downstream height, the fluid jet velocity, and gravity. Of these, gravity is the most poorly understood and no experimental studies have been reported concerning its effect on the CHJ diameter. Gravity also influences the jump profile shape which in turn influences heat transfer around the jump.

Progress During FY 1996:

Research pursued over the past year was carried out under a no-cost extension to this grant. A package was designed and fabricated to house an orifice jet, circulating pump, and cameras for observing a CHJ in microgravity. The components are the following: recirculating pump; plenum containing beads and a flow straightener (to dampen the inlet flow) and a removable orifice plate attached at one end; Plexiglas chamber within which the target plate is mounted; flow control valve; and cameras and lighting. The experimental design allows views of the impinging jet from the top, the side (i.e., along the plane of the spreading film to observe the profile shape across the jump) and from underneath. The height of the liquid level downstream of the jump was controlled by submerging the target plate to the desired depth. Experiments were carried out for downstream heights of 2.0 mm, 4.0 mm, 6.0 mm, 10.0 mm, or 15.0 mm. The liquid flow rates were 2.39ml/s, 6.32ml/s, 9.93ml/s, or 26.47ml/s. The evolution of the CHJ diameter was recorded during the transition from $G=1$ to $G\ll 1$ by a CCD camera operating at about 30 frames/s, and a 35mm camera operated at 5 frames/s. From the video and photographic images obtained, the variation of CHJ radius and profile shape with time were determined from a frame-by-frame analysis using a computer based image-analysis system.

Results of the experiments and analysis of the results are the following: 1) a steady CHJ can be established in microgravity; 2) the CHJ in microgravity is larger than at normal gravity, other flow conditions being equal; 3) the fluid response time during the transition to microgravity is on the order of 200ms when a jump exists at normal gravity; 4) when flow conditions are such that a CHJ does not exist at normal gravity, the fluid response time appears to be greater than 1s after the transition to microgravity; 5) the film thickness across the CHJ boundary at $G \ll 1$ is more gradual than at $G=1$ due to the reduction in hydrostatic pressure in the downstream film at $G \ll 1$, and 6) while the $G=1$ measurements are well correlated by an existing formulation, the microgravity measurements show comparatively poorer agreement.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/94 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-24-05-34

NASA CONTRACT NO.: NAG3-162

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Avedisian, C.T. and Zhao, Z., "The hydraulic jump in microgravity. J. Fluid Mech., (1996).

Presentations

Avedisian, C.T. and Zhao, Z., "Experimental study of liquid jet impingement in microgravity: the hydraulic jump." 3rd Int. Microgravity Fluid Physics Conf., Cleveland, June 12-14 ,1996.

Numerical Simulation of Electrochemical Transport Processes in Microgravity Environments

PRINCIPAL INVESTIGATOR: Prof. Sanjoy Banerjee

University of California, Santa Barbara

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Electrochemical processes are used in space for a variety of purposes, such as the generation of oxygen for life support, and the production of hydrogen for propulsion and energy storage. In space, these gases are generated at the electrode wall and tend to accumulate, due to the lack of gravity-driven buoyancy that typically would 'clear' the wall. This behavior reduces the electrical efficiency of electrochemical cell, since electrolyte is from the electrode. The main objective of this work is to determine the parameters that control the growth and detachment of gas from the electrode wall. This work will also investigate the role of turbulence in the transfer of electrolyte to the electrode surface and for the removal of the gas phase at the surface.

Task Description:

Task Significance:

This work has applications in many flows of engineering interest, where a dispersed phase interacts with a fluid undergoing turbulent flow. For example, the entrainment of gas bubbles in the wake of a ship has been shown to contribute to the long streaks observed behind the ship.

Since this work is numerical in nature, new computational techniques must be developed to track the interfaces of the dispersed phase. Current techniques are limited to 'well-behaved' bubbles (i.e. bubbles that don't break apart), interacting with laminar flows. The numerical techniques used in this work will be able to simulate the interaction between turbulent flows and multiple, breaking bubbles.

Progress During FY 1996:

This is a new project just started in May, 1996. One of the PI's Ph.D. student has already begun formulating the equations describing the interactions between the electrolyte and the bubbles inside the electrolyte.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-185

RESPONSIBLE CENTER: LeRC

Control of Flowing Liquid Films by Electrostatic Fields in Space

PRINCIPAL INVESTIGATOR: Prof. S. G. Bankoff

Northwestern University

CO-INVESTIGATORS:

Schluter
MiksisNorthwestern University
Northwestern University**Task Objective:**

An objective of this work is to demonstrate experimentally that electric fields can be employed to repair punctured flowing liquid films in low gravity. A second objective is to improve the theoretical tools needed to predict behavior of systems that will work experimentally. This work will support the development of Electrostatic Liquid Film Radiators for space-based heat management applications.

Task Description:

There are experimental and theoretical efforts in this work.

The experiments are earth-based using a carefully oriented vertical plate to avoid g-forces normal to a film flowing on the plate surface. The plate will have a hole in it over which the fluid will flow. A transparent flat electrode will be positioned parallel to the film and the hole in the plate. This assembly will be placed inside a vacuum bell jar where a small differential pressure can be applied across the fluid spanning the hole in the plate. Large electric fields can be applied between the electrode and vertical plate to apply forces to the liquid film. Visual viewing of the film flowing over the hole is provided. The procedure will require inducing a rupture with no electric field present using the differential pressure across the film. Then in the absence and presence of a several electric field strengths the differential pressure is adjusted until the rupture is healed.

The theoretical work will start by calculating the film free surface shape for a dielectric fluid, which will be used in the experiments. The case of a conducting fluid has been done previously. After that free surface calculation is complete the coupling of the electrostatic field distribution to the fluid film motions and thickness will be numerically modeled.

Task Significance:

This work will improve engineering choices regarding Electrostatic Liquid Film Radiators for space-based heat management designs.

Progress During FY 1996:

A vacuum system having an 18" x 24" working space with eight access ports has been assembled and is working. The mechanical fore-pump produces a vacuum of less than 20 millitorr. A 6" diffusion pump brings the pressure down to less than 0.01 millitorr in 5 minutes, well up on the vacuum side of the Paschen curve of dielectric strength vs residual gas pressure, corresponding to a breakdown electric stress of approximately 10 MeV/meter. Pressure instrumentation to work in the intended pressure range are installed (two "convectrons"). A cold trap on the input side of the pump is installed and is available if necessary to keep diffusion pump oil molecules out of the experimental space.

A 30 KeV high voltage power supply has been obtained and the high voltage system is in process of assembly. Detection and monitoring of possible leakage or breakdown currents is provided by a meter and also a battery-operated oscilloscope that is isolated and can measure the supply conductor to the high voltage entry port of the experiment.

A Wild/Leica theodolite has been obtained which will be used to maintain exact verticality of the fluid flow wall. Optical ports will allow sighting the surface from both sides.

Fabrication is in progress on the separate space on the "outside" of the putative leak hole, a space in the form of a tube projecting into the main space. This space must have separate sensitive pressure controls and optical access to

the hole in order to measure features of leakage flow. This tube will bear the hole mount. Calibrated holes (relatively economical items made for laser research) are on order.

Study is in progress on a small gear pump to mount inside to move the fluid. It, and all other features of the system, must be free of vibration, a requirement set by extraneous acceleration of the flow plane to be less than 1 micro-g in the frequency range from 1 to about 1000 hertz which might influence the motion of the fluid.

Design is proceeding on the tubing network involving the valves, the differential pressure sensor, and the gas source, and vacuum access.

STUDENTS FUNDED UNDER RESEARCH:		TASK INITIATION:	9/96	EXPIRATION:	5/00
BS Students:	0	PROJECT IDENTIFICATION:	962-24-00		
MS Students:	0	NASA CONTRACT No.:	NAG3-185		
PhD Students:	1	RESPONSIBLE CENTER:	LeRC		

Forced Oscillation of Pendant and Sessile Drops

PRINCIPAL INVESTIGATOR: Dr. Osman A. Basaran

Purdue University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objectives of the proposed research are to develop a fundamental understanding of forced oscillations of supported drops and to clarify in particular the effects of surface-active species and the type of driver in such driven oscillations.

Task Description:

The research will be accomplished through the following tasks and subtasks:

1. Analyze through computation and experiment, the oscillations of a pendant/sessile drop which is surrounded by a gas and supported on a rod or a wall, that is forced to oscillate sinusoidally in time.

Determine the response of a drop with a fixed contact line (FCL) and a clean interface.

Study the response of a drop with a fixed contact line (FCL) and in the presence of surface-active species;

- insoluble surfactant
- soluble surfactant

Study the response of a drop with a moving contact line.

2. Develop through computation and experiment, a qualitative and quantitative understanding of the effect of the driver on the oscillations of a pendant/sessile drop which is surrounded by a gas and supported on a rod or emanating from a capillary tube.

Determine the response of a drop forced to oscillate by a time-periodic electric field;

- conducting drop
- insulating drop

Determine the response of a drop forced to oscillate by varying sinusoidally in time the flow rate in the tube.

Task Significance:

An improved understanding of forced oscillations of supported drops is needed in areas as diverse as (a) electric field-enhanced multiphase separations, (b) electro-atomization techniques for the synthesis of ceramic precursor powders, (c) growing of pure crystals in low-gravity, and (d) the pulsating bubble technique for measuring dynamic surface tension. In (a) and (b) the energy required to break up or atomize supported drops can be minimized by taking advantage of the resonant coupling that can occur between the natural oscillations of the drop and the oscillations of the driver. In (c), it is important to understand the effect of support vibrations on the quality of grown crystals, e.g. in a low gravity environment. In (d), a bubble that is pendant from a tube and is surrounded by a surfactant solution is forced to undergo oscillations to infer the dynamic surface tension of the interface.

The research effort proposed here conforms with several program objectives and addresses issues in several research categories of interest to the Microgravity Science and Applications Division (MSAD). In particular, the area of "capillary phenomena" while touching on areas including "convective phenomena", "electrokinetics and electrochemistry", "thermocapillary and solutocapillary phenomena" and "crystal growth." Furthermore, the oscillation of drops is a problem of general engineering and scientific interest, with a history dating back to the works of such giants of the 19th century such as Lord Rayleigh and gaining importance in recent years because of applications in technology and to the field of nonlinear science.

Progress During FY 1996:

This is a new grant which was awarded in June 1996. The hiring of graduate students and technicians has been accomplished. Equipment for the model (mostly computer related) has been purchased. Initial grant work is now underway.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 2
PhD Students: 0

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-186

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

DePaoli, D.W., Basaran, O.A., Feng, J.Q., and Scott, T.C., Forced oscillations of pendant drops. Sep. Sci. Tech., (accepted 1996).

DePaoli, D.W., Feng, J.Q., Basaran, O.A., and Scott, T.C., Hysteresis in forced oscillations of pendant drops. Phys. Fluids, (accepted 1996).

*Studies on the Response of Emulsions to Externally-Imposed Electric and Velocity Fields:
Electrohydrodynamic Deformation and Interaction of a Pair of Drops*

PRINCIPAL INVESTIGATOR: Dr. James C. Baygents

University of Arizona

CO-INVESTIGATORS:

Stone, H.

Harvard University

Task Objective:

The objective of this study of multiphase electrohydrodynamic flows is to determine the electric field-induced microstructural response of two-phase systems, as well as to develop an improved understanding of the physico-chemical and transport process common to a variety of low-gravity flows; we examine the motion, deformation, and interaction of pairs of viscous drops owing to an applied electric field.

Task Description:

The research is a comprehensive numerical and theoretical study of several phenomena common to multiphase flows where electrical fields are used to manipulate the microstructure in the absence of any buoyancy-induced fluid motions. This class of problems appears in typical materials handling, physico-chemical processes (e.g., emulsion breaking and drop coalescence) and bioseparations processes (e.g., aqueous two-phase partitioning).

This investigation is designed to use numerical solutions to develop an improved quantitative understanding of the effect of electric fields on typical two-drop (pair) interactions that lead toward coalescence. Cases will be studied where the potential distribution is influenced by conduction processes in the limit where viscous effects dominate the hydrodynamics. Both the effects of uniform and simple nonuniform (imposed) fields will be studied. The "leaky" dielectric model and the Stokes equations will be employed to describe the constitutive behavior of the dielectric media. The numerical calculations will use established integral equation methods for solving this class of time-dependent free boundary problems.

Task Significance:

The systematic study will lead to a quantitative description and understanding of electrically-driven low-gravity fluid motion, particularly as these flows pertain to the manipulation and positioning of drops and bubbles with electric fields. Such flows are significant for several reasons. First, in the absence of the usual gravitational forces, electric fields can be used to effect phase separation processes that are controlled by drop coalescence (e.g., emulsion breaking). Second, electric fields have long been envisioned as a tool for containerless processing of materials, inasmuch as the fields can be used to manipulate fluid interfaces, such as those of a drop surface, and as a means to levitate fluid globules against weak gravitational fields.

Progress During FY 1996:

The significant milestones for 1996 are:

1. development of an expression for the force and torque on an isolated body in an electric field that varies linearly with position.
2. development of an analytical expression for the axisymmetric, electric-field driven relative motion between a pair of leaky dielectric spheres.
3. development of a boundary integral code for the translation, deformation and rupture of a leaky dielectric drop in an electric field that varies linearly with position.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	2	MS Degrees:	1
PhD Students:	0	PhD Degrees:	0

TASK INITIATION: 3/93 **EXPIRATION:** 3/96

PROJECT IDENTIFICATION: 962-24-08-13

NASA CONTRACT NO.: NAG8-948

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Baygents, J.C., Rivette, N.J., and Stone, H.A. Electrohydrodynamic deformation and interaction of drop pairs in viscous fluids. *J. Fluid Mech.*, accepted, (1996).

Rivette, N.J. and Baygents, J.C. A note on the electrostatic force and torque acting on an isolated body in an electric field. *Chem Eng. Sci.*, vol. 51, 5205-5211 (1996).

NASA Tech Briefs

Erker, J.A. and Baygents, J.C. Electrohydrodynamic interaction of a pair of spherical drops. NASA Conference Publication 3338, 731-735 (1996).

Dynamics of Granular Materials

PRINCIPAL INVESTIGATOR: Prof. Robert P. Behringer

Duke University

CO-INVESTIGATORS:

Thompson, P.A.

Duke University

Task Objective:

This project entails the study of how gravity affects the dynamics of shaken granular materials. There are several motivations for this work. In particular, the dynamics of granular materials is highly important to a broad range of technical, agricultural, and pharmaceutical processes involving many billions of dollars annually in the United States.

Task Description:

The task consists of a detailed characterization of the dynamics of shaken granular materials. Experiments will identify important behavior and flow properties for shaken granular materials. Shaking will be carried out both vertically and horizontally.

Task Significance:

The shaking of granular materials is particularly important as a tool to transport and process a variety of materials. Gravity plays an intrinsically important role in this case. Looking into the future, attempts to mine on the lunar surface will almost surely involve shaking processes for granular materials.

Because our understanding of granular flows is rather poor, many of the plants and devices which handle granular materials operate significantly below capacity, and fail all too frequently. The result is corresponding loss to the US economy.

Progress During FY 1996:

The project will focus on the dynamics of these materials. To date we have 1) identified, using an existing apparatus, a novel instability which leads to waves in shaken granular materials--a manuscript has been submitted to the journal of Physics Letters A; and 2) constructed a novel laboratory shaking apparatus which can provide independent motion in both the vertical and horizontal directions. This apparatus also can fluidize the gas, which is a related and technically important process (i.e. for the burning of coal, etc.) We are now studying the flow states of this system using both conventional and high-speed video techniques.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	1
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 7/96 EXPIRATION: 7/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-191

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Tennakoon, S. and Behringer, R.P. Onset of flow for horizontally shaken granular materials. Phys. Rev. E., (submitted, 1996).

Investigation of Drop Formation by a Vortex Ring in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Luis P. Bernal

University of Michigan

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this study is to examine the dynamics of drop formation by vortical flows at the capillary limit of moderate or high Weber Numbers and infinite Froude Numbers.

Task Description:

Experiments will be conducted in the NASA LeRC 2.2 Second Drop Tower to determine the effect of Weber and Reynolds Numbers in the formation of single and multilayered liquid drops in air. In addition, testing will be conducted at the University of Michigan using equal-density, immiscible fluids. Velocity fields will be measured using Particle Image Velocimetry. Numerical simulation of the flows will be conducted using a front-tracking method using the full Navier-Stokes equations for axisymmetric flow conditions.

Task Significance:

The purpose of this study is to achieve a better understanding of the role of vorticity at either a gas-liquid or liquid-liquid interface on drop formation. Modeling fluid atomization and microencapsulation processes is important towards developing an understanding of two-phase (gas-liquid) flow in pipes to assist in the design of space-based power and thermal management systems and of terrestrial-based nuclear power plants and oil and natural gas pipelines.

Progress During FY 1996:

The effort has focused on the design for the reduced gravity experiment, and the PIV data processing and system development for the normal gravity equal-density, immiscible fluids testing. A conceptual design was prepared and critiqued by the Drop Tower personnel, and a drop tower frame was forwarded to the PI. Preliminary normal gravity experiments were conducted with a Bond Number range of 0.05 - 3.9, a Weber number range of 2 - 100, and a viscosity ratio range of 1 - 5. Preliminary PIV measurements were also obtained for the single liquid layer.

The results of these preliminary observations show the complex nature of the drop formation process. The location of the interface breakup and formation of smaller satellite drops have been documented. The minimum Weber number for drop formation to occur has been found. The PIV data is being processed to compare with the relevant theories of vortex ring propagation in an unbound fluid.

The results obtained from these observations suggest that vorticity dynamics at the interface plays a key role in the formation of the satellite drops. This is a new result that should be incorporated in the theoretical analysis of atomization in vortical flows. These results are also being used to further define the reduced gravity experiments.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NCC-3-47

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Bernal, L.P. and Maksimovic, P., "Investigation of drop formation by a vortex ring in microgravity." paper presented to The Third Microgravity Fluids Physics Conference, NASA, Cleveland OH, publication 3338, pp 501-508, June 13-15, 1995.

Dynamic Modeling of the Microgravity Flow

PRINCIPAL INVESTIGATOR: Dr. Jeremiah U. Brackbill

Los Alamos National Laboratory

CO-INVESTIGATORS:

Kothe, D.B.

Los Alamos National Laboratory

Task Objective:

The objectives of our numerical modeling project are to improve existing algorithms for modeling interfacial flows, to improve modeling capabilities in three dimensions, and to apply computer modeling to physics issues, including surface-tension-driven flow, boiling and mixing, and the possible role of electric fields.

Task Description:

To meet our objectives, we have organized our research along three, complementary lines; analysis, implementation, and the definition and solution of physical problems by numerical modeling. Through analysis, we seek to eliminate parasitic currents and reduce the cost of calculations that include surface tension and other stiff terms. Parasitic currents are flows of numerical origin that persist long after equilibrium should have been achieved. They are due to the absence of energy conservation, and their suppression requires the definition of an appropriate energy integral. Surface tension supports capillary waves, whose fast propagation speed limits computational time steps to very small values. Implicit formulations of the surface tension contribution can be very useful in reducing the cost of computations when it is unnecessary to resolve capillary waves.

Through careful implementation of algorithms for interfacial physics, we will leverage the development of three-dimensional modeling capabilities for concurrent processors to achieve the resolution needed to model complex flow problems. Physical problem definition will be carried out through strategic partnerships with others in the microgravity program. We hope also to solve physical problems through collaboration.

Task Significance:

The ultimate contribution of this project is a better fundamental understanding of microgravity flows and their interaction with interfacial phenomena driven by surface tension, wall adhesion, and phase changes. Computational modeling in collaboration with theoretical and experimental studies will offer new insight into these processes on the small scale, and can provide guidance to the design of safe and efficient fluid storage and heat transfer devices, and in the development of advanced material processes.

Progress During FY 1996:

An implicit surface tension algorithm has been developed which requires the solution of a single potential-like equation to remove the capillary time step constraint. Variational forms of the continuum surface force for which there is an energy integral have been derived.

A second-order volume-of-fluid surface reconstruction has been developed and implemented in three dimensions. The results of many tests indicate the method is accurate and robust, and a promising vehicle for additional interfacial physics.

Other Participants:

Damir Juric, who received his Ph.D. under the supervision of Gretar Tryggvason at the University of Michigan, has joined the project, his thesis research includes problems in solidification and boiling.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/97

PROJECT IDENTIFICATION: 962-24-00

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Brackbill, J.U., and Kothe, D.B., "Dynamical modeling of surface tension." Third Microgravity Fluid Physics Conference, NASA Lewis, Cleveland, June 1996.

Juric, D. and Tryggvason, G., "Direct numerical simulations of flows with phase change." AIAA 96 0857, 34th AIAA Aerospace Sciences Meeting, 1996.

Juric, D. and Tryggvason, G., "Computations of fluid boiling, in advances in numerical modeling of free surface and interface fluid dynamics." FED-vol. 238, ASME, pp. 341-347, 1996.

Kothe, D.B., Rider, W.J., Mosso, S.J., Brock, J.S., and Hochstein, J.I., "Volume tracking of interfaces having surface tension in two and three dimensions." 34th Aerospace Sciences Meeting & Exhibit, AIAA, Reno NV, AIAA 96-0859, 1996.

Marangoni Effects in Boiling of Binary Fluid Mixtures Under Microgravity

PRINCIPAL INVESTIGATOR: Prof. Van P. Carey

University of California, Berkeley

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Recent efforts to more fully optimize performance of power, refrigeration and thermal control systems have lead some developers to consider the use of binary working fluids. Vaporization of the working fluid is often a critical element in the performance of such systems. However, transport phenomena associated with vaporization of binary liquid mixtures is still not well understood. The main objective of this project is to separate and explore the roles of buoyancy and Marangoni effects in binary liquid mixture boiling under simulated low gravity conditions. The research will also aim to find coolant mixtures that are particularly well suited for use in a variety of applications including spacecraft thermal control.

Task Description:

This project consist of a series of experimental studies of nucleate boiling of a variety of binary mixtures. The experiments will include both 1-g and low-g data of boiling curve and critical heat flux. Testing the boiling performance of the heating surface in different orientations will establish whether the presence of Marangoni effects reduces the sensitivity of the system to the direction of the gravity vector. The least sensitive mixtures will then become the focus of tests under low gravity conditions (via NASA low-g aircraft).

Task Significance:

The experimental database for boiling of binary fluid mixtures will help to clarify the individual contributions of gravity and Marangoni effects on the heat transfer from the surface and the critical heat flux transition. It will also help to develop a capability to model these effects with reasonable accuracy to improve the designs of thermal systems.

Progress During FY 1996:

In September and October of 1995, the test apparatus was prepared for flight testing. It was shipped to NASA Lewis in November and flight experiments were conducted on the DC-9 aircraft in early December of 1995. Some additional 1-g experiments were conducted in our laboratory after the test apparatus was returned to Berkeley in February of 1996. During the period from February 1996 to August 1996, the data from the experiments was analyzed and technical papers based on them have been drafted.

The flight experiments provided boiling heat transfer data and high speed video recordings of the boiling process for mixtures of water and propyl alcohol at pressures ranging from 5.5 to 9.5 kPa. The alcohol mole fraction in these experiments ranged from about 0.015 to 0.1. This variation was selected to cover mixtures with different levels of Marangoni effects. In each experiment boiling heat transfer data was obtained for acceleration levels less than 0.01g and approximately 2g (during the climb between free-falls). Experiments over the same parameter ranges have also been conducted at 1g in our laboratory at Berkeley. The data clearly demonstrate that delivery of liquid to the surface by surface tension gradients can sustain the boiling process under low gravity conditions. These data are now being compared with predictive correlations and other binary mixture boiling data in the literature. The results of these comparisons will be included in the forthcoming technical papers and final report summarizing the findings of these studies.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/94 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-24-05-81

NASA CONTRACT No.: NAG3-163

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Ahmed, S., Carey, V.P., and Motil, B. "Marangoni effects in the boiling of binary fluid mixtures." Third Microgravity Fluid Physics Conference, Cleveland, OH, June 13-15, 1996.

Marangoni Instability Induced Convection in Evaporating Liquid Droplets

PRINCIPAL INVESTIGATOR: Dr. An-Ti Chai

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

Arpaci, V.R.

University of Michigan

Task Objective:

The objectives of the proposed effort are: (1) to study and to characterize the Marangoni instability phenomena in the near ideal configuration of an evaporating droplet in microgravity, and (2) to establish the effect of the induced convection on the droplet evaporation rate.

Task Description:

Specifically, the purpose is to study the Marangoni instability and thermocapillary convections in an evaporating liquid drop in the Fluids Experiment System (FES) developed for flight on Space Shuttle missions. However, the proposed flight experiment was redirected to proceed as a ground-based project with emphasis on refining the theoretical model. Different numerical methods and techniques are tested and evaluated for the case of evaporating droplets.

Task Significance:

When the proposed experiments are successfully completed, the unique data set, which will be collected under near ideal conditions, should by itself constitute a significant contribution to our knowledge of droplet evaporation. The significance and influence of the proposed project go far beyond any unique experimental data set. With the anticipated data set, it will be possible to quantitatively evaluate the well known Maxwell's theory of droplet evaporation. Additionally, it will be possible to establish that thermocapillary instability induced convection inside a droplet can affect its evaporation process. It is our intention to use this information to pursue the development of a complete and comprehensive theory of droplet evaporation.

The value of a more comprehensive and complete theory cannot be overstated. Having a solid theoretical basis, numerical computation can be devised along with skillful scaling techniques to explore cases where direct experimentation is not feasible. The influence of the proposed work is expected to be far reaching in this regard.

Progress During FY 1996:

Experimental Effort: A proposal to conduct Glovebox experiments on "Droplet Injector and Evaporation" was submitted and a review for the final selection was conducted in February 1996. Although our Glovebox experiment was not selected for flight, we did accomplish the following:

1. Received funding for Glovebox selection review.
2. Prototype injectors of different sizes have been fabricated for both bench test and Zero-G drop test to demonstrate feasibility.
3. Both manual and automated mode of operation of the injector were studied.
4. Alternate injector designs were considered and tested.
5. Various evaporating sample liquids were evaluated.
6. Conducted limited DC-9 tests and Zero-g tests.

Theoretical Effort: In the past two years we have tried the projection method for the instability of evaporating horizontal layers. First, we tested the method in the absence of evaporation. We then included the effect of evaporation; the results were presented at the 9th International Conference on Numerical Methods in Laminar and Turbulent Flow in Atlanta.

The use of the "Projection Method" for deforming droplets does not appear to be feasible. This year Professor Arpaci successfully tested the front tracking method for the dynamics of interface mechanics in general and for the evaporating droplets in particular. Preliminary results will be analyzed and reported later. Separately, we are trying to apply the chaos theory to the second transition of the thermocapillary instability of horizontal layers. However, the method is only applied for the case of no evaporation.

Special effort has been put forward by Professor Arpaci in search for the Kilmogorov microstructure of the interface dynamics. It is expected that this structure should be related to the wavelength of the growing disturbances. The following three keynote lectures on the microstructure of turbulence have been presented at international conferences: 1) 10th International Heat Transfer Conference at Brighton, England, August 14-18, 1994, 2) The International Symposium on Turbulence, Heat and Mass Transfer at Lisbon, Portugal, August 8-12, 1994, and 3) Third Latin-American Symposium on Fluid Mechanics at Caracas, Venezuela, February 5-8, 1995.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 4/93 **EXPIRATION:** 4/96

PROJECT IDENTIFICATION: 962-24-05-65

NASA CONTRACT NO.: NAG3-113

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Chai, A-T. and Zhang, N., "Marangoni-Benard convection in an evaporating liquid thin layer." The Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 13-15, 1996.

Esmaeeli, A., Arpaci, V.S., Chai, A.T., "Direct numerical simulations of evaporating droplets." Second European Symposium on Fluids in Space, Naples, Italy, 22-26, 1996.

Kao, S-H, Arpaci, V.S., and Chai, A-T., "Thermocapillary driven flow past marangoni instability." Second European Symposium on Fluids in Space, Naples, Italy, 22-26, 1996.

Marangoni Instability Induced Convection in Evaporating Liquid Droplets

PRINCIPAL INVESTIGATOR: Dr. An-Ti Chai

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

Arpaci, V.R.

University of Michigan

Task Objective:

The objectives of the proposed effort are: (1) to study and to characterize the Marangoni instability phenomena in the near ideal configuration of an evaporating droplet in microgravity, and (2) to establish the effect of the induced convection on the droplet evaporation rate.

Task Description:

The original proposal was intended as a flight experiment proposal; however, NASA Headquarters program office has decided to redirect the proposed effort to ground-based investigation. We have adjusted our FY 1996 Tasks accordingly.

Ground-Based Experiment Tasks:

1. To investigate the effects of evaporation on instabilities and thermocapillary flows in a thin liquid layer.
2. To continue drop tower testing of droplet & bubble injection devices.

Modeling Tasks:

1. To work on the front tracking/finite difference formulation of evaporating liquid droplets.
2. To simulate numerically thermocapillary flows in a thin evaporating liquid layer.

Task Significance:

Recent experimental results demonstrated that evaporation can have significant effects on instabilities and thermocapillary flows in a thin liquid layer. The traditional theory of linear instability simply can not explain what we have observed. We intend to further investigate the mechanism of evaporation and how it interacts with the thermocapillary phenomena of interests. Modeling task (2) is added to help accomplishing that goal.

Progress During FY 1996:

This is a new task which just started in July, 1996. Experiment results show that evaporation has a key effect on thermocapillary convection in an evaporating thin layer. Berard cells can be sustained by the evaporation in a thin layer with a nonlinear temperature profile and even with zero or a positive temperature gradient when the layer is cooled from below. Traditional theories and mechanism model can not explain these phenomena. A surface-tension driven convection mechanism which relates the thermocapillary convection to evaporation is presented. The boundary condition on surface of the evaporating layer was analyzed, and a new expression of Marangoni number is suggested to describe the instability and status of the evaporative convection.

Progress is being made to implement a two-dimensional front tracking/finite difference technique for fluid flows with phase change:

- Formulation modified to take into consideration of the energy jump and the interface boundary conditions.
- Simulation results have been compared with analytical solution of a simple one-dimensional problem; good agreement have been obtained.
- In the iteration scheme, the predetermined convergence factor has been changed into an adaptive one. This has resulted in a faster convergence rate.
- Thermocapillary effects are being investigated in selected problems.
- Code has been modified to study the multibubble dynamics.
- An algorithm has been implemented, which allows the fronts to coalesce once they are closer than a critical distance.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/96 EXPIRATION: 9/00

PROJECT IDENTIFICATION: 962-24-00

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Books

Zhang, N. and Chai, A.-T. "Effects of Evaporation on Thermocapillary Flows in a Liquid Thin Layer," in "Heat Transfer Science and Technology." Edited by: Wang Buxuan Higher Education Press, Beijing, China, pp 329-334, 1996.

Rewetting of Monogroove Heat Pipe in Space Station Radiators

PRINCIPAL INVESTIGATOR: Prof. S. H. Chan

University of Wisconsin, Milwaukee

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The general objective of the program is to investigate the physics of rewetting of heated, grooved flat plates in a microgravity environment.

Specific objectives of the program are to add to the fundamental understanding of the physics of rewetting/dryout fronts; to better quantify the conditions under which rewetting occurs; and to obtain more accurate predictions of the rewetting velocity for a range of parameters.

Task Description:

The program is composed of both experimental and theoretical investigations. For the experimental investigation a grooved flat plate apparatus will be designed and constructed. Liquid will be introduced on one side of the plate to flow along the grooved surface; the other side of the plate will be electrically heated. This apparatus will be operated both on the ground and aboard a microgravity aircraft.

Data from these experiments will consist of temperature measurements in the liquid film and the heated plate. Advancing wetting front (rewetting), receding wetting front (dryout), and stationary wetting front cases will be examined.

The theoretical analysis will be made by applying experimental data on rewetting velocity and temperatures to analytical processes developed for predicting rewetting velocities on overheated nuclear fuel rods.

Task Significance:

Understanding the dryout and rewetting characteristics of grooved surfaces is important in predicting behavior of monogroove heat pipe designs proposed for the space station.

Progress During FY 1996:

Considerable progress has been made on fundamental studies of rewetting of heated, capillary grooved surfaces. The accomplishments made in the fiscal year of 1996 are listed below:

1. **Rewetting Experiments in Simulated Gravity Conditions:** Simulating experiments in a normal gravity environment to investigate gravity effects on rewetting of capillary grooved surfaces have been made. Specifically, the rewetting experiments of a uniformly heated grooved surface in both downward facing and upward facing conditions have been performed. It was found that, for a rewetting fluid of 2-propanol, the rewetting temperature was 93–96°C for the upward-facing case and about 2°C lower for the downward facing case. When the initial plate temperature was higher than the rewetting temperature, the rewetting speed decreased with the initial plate temperature. The rewetting speed is also faster in the upward-facing case than in the downward-facing case for the same initial plate temperatures, which indicates a gravitational effect on rewetting. This trend is found to be consistent with the previously investigated end heating condition.
2. **Rewetting Theoretical Development:** The rewetting models developed by the author and his coworkers, which were reported in previous progress reports, have been applied to predict the rewetting distance versus time for the grooved plate subjected to uniform heating. The predicted rewetting distances were found to be in fair agreement with experimental data, with maximum discrepancies of about 20%. Both experimental and calculated results show that the transient rewetting distance increases with the plate initial temperature when the initial temperature is less than the rewetting temperature. But when higher than the rewetting temperature, the rewetting distance decreases with the increasing initial plate temperature.

3. Drop Apparatus Design and Reduced Gravity Experiments: Prior to investigate the rewetting behavior in a reduced gravity environment in an aircraft, it is prudent that components of the tested loop to be used in the aircraft be tested in a drop apparatus for safety, functionality and resilience. To this end, a drop tower, which allows experiments to be conducted in an inertial frame, has been built and is functional. This inertial frame experiences an average relative acceleration of ~ 0.1 g for about 0.9 seconds. The drop tower apparatus are being used to test a reservoir design integrated with a test section, and with their controlling mechanisms and associated instrumentation accessories. Experiments are also being conducted to test rewetting speed on a heated, capillary grooved surface under such reduced gravity conditions.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	0
MS Students:	2	MS Degrees:	1
PhD Students:	0	PhD Degrees:	0

TASK INITIATION: 12/92 EXPIRATION: 12/97

PROJECT IDENTIFICATION: 962-24-05-54

NASA CONTRACT NO.: NAG3-138

RESPONSIBLE CENTER: LeRC

Marangoni and Double-Diffusive Convection in a Fluid Layer Under Microgravity

PRINCIPAL INVESTIGATOR: Prof. Chuan F. Chen

University of Arizona

CO-INVESTIGATORS:

Chan, C.

University of Arizona

Task Objective:

To study salt-finger convection in a stratified fluid layer due to thermal and solutal capillary motion.

Task Description:

A coordinated research effort in ground-based experiments, stability analysis, and numerical simulations is applied to study salt-finger convection induced by combined thermal and solutal capillary motion. Experiments are conducted in a stratified fluid layer to suppress or reduce buoyancy effects encountered under Earth gravity. Numerical simulations are conducted by developing a finite difference code. Once validated by the experimental results, the numerical code will enable us to predict the outcome under microgravity.

Task Significance:

The results of this study will enable the design of an apparatus for crystal growing and for casting in a space environment. In addition, it will offer an improved understanding of materials processing, which will enhance the chances of obtaining new and better quality crystals for the semiconductor industry and for the biomedical industry. This study can also provide an improved understanding of the interaction of surface tension forces and double-diffusive buoyancy forces, which would lead to the improvement of manufacturing processes on Earth.

Progress During FY 1996:

Experiments were conducted in both a deep (5 cm x 10 cm x 10 cm deep) and a shallow (5 cm x 10 cm x 1 cm deep) tank. The test fluid was a stratified ethanol-water solution with pure ethanol at the upper free surface. A stable density gradient was established at approximately 4 wt% water/cm at the beginning of the experiment. In both tanks, when a temperature difference of 2°C was imposed at the two side walls, capillary motion was generated, bringing heavier fluid above the lighter fluid. Finger convection was soon generated near the cold wall in the form of longitudinal rolls, which gradually filled the tank.

Numerical simulations show that, when the temperature difference is first imposed, a vortex at both the heating and cooling walls is generated by thermocapillarity. These vortices bring fluid with a higher water concentration to the free surface, thus generating solutal capillarity, which enhances (retards) the thermocapillarity near the cold (hot) wall. Consequently, the vortex near the hot wall decays while the vortex near the cold wall grows, which greatly distorts the temperature and concentration fields. This explains why the finger convection, contrary to intuition, starts near the cold wall. Further experiments and numerical solutions are planned to obtain a better understanding of the three-dimensional flow field.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 3

TASK INITIATION: 12/92 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-24-05-51

NASA CONTRACT NO.: NAG3-138

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Jin, Y. Y., and Chen, C. F., Stability of convection and heat transfer of high Prandtl number fluids in a vertical slot. *J. Heat Transfer*, vol. 118, pp. 359-365 (1996).

Jin, Y. Y., and Chen, C. F., Natural convection of high Prandtl number fluids with variable viscosity in a vertical slot. *Int. J. Heat Mass Transfer*, vol. 39, pp. 2663-2670 (1996).

Jin, Y.Y. and Chen, C.F., Effect of gravity modulation on natural convection in a vertical slot. *Int. J. Heat Mass Transfer*, (May 1996).

Tanny, J., Chen, C.C., and Chen, C.F., Interaction between Marangoni and double - diffusive instabilities. *J. Fluid Mech.*, vol. 303, pp. 1-21 (1995).

Proceedings

Chen, C.F., "Particle flux through sediment fingers." *Proceedings of the 12th Australasian Fluid Mechanics Conference*, Sydney, Australia, pp. 171-174, December 10-15, 1995.

Chen, C.F. and Chan, C.L., "Salt-Finger convection in a stratified fluid layer induced by thermal and solutal capillary motion." *Proceedings of the NASA 3rd Fluid Physics Conf.*, NASA Lewis Research Center, June 13-15, 1996.

Presentations

Chen, C.F., "Particle flux through sediment fingers." 48th Annual Meeting of APS - DFD, University of California, Irvine, November 1995.

Transport Phenomena in Stratified Flow in the Presence and Absence of Gravity

PRINCIPAL INVESTIGATOR: Prof. Norman Chigier

Carnegie Mellon University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The strategy of this study is as follows:

1. To separate the effects of molecular and turbulent diffusion from gravitational forces during the mixing of two shear layers.
2. To identify the relevant and characteristic non-dimensional parameters that govern the physical interaction between fluid layers in the range of the proposed experimental conditions.
3. To examine the interaction between buoyant plumes and stratified shear layers, and to study the rates of entrainment into buoyant plumes and stratified shear layers.
4. To study the effects of injecting solid and liquid particles into fluid streams under stable and unstable stratified shear flow conditions.
5. To identify potential instrumentation that could distinguish between molecular and turbulent diffusion in the presence and absence of gravity.

Task Description:

1. Conduct detailed measurements in turbulent mixing layer with velocity and density gradients.
2. Conduct a scoping on the interaction of buoyant heated jets and plumes interacting with stable and unstable stratified shear layers.
3. Develop scaling laws and similarity criteria for comparison with measurements made in the "main" and "reduced" scale experiments.

Task Significance:

To use the reduced gravity environment to improve the understanding of the fundamental physical processes of mixing between layers of fluids of different densities and velocities. The following are a few matters that are important to this research project:

1. To understand the process of dispersion of pollutants in a highly stable stratosphere and in outer space.
2. To understand the effect of dispersion of pollutants emitted from a space craft at high altitudes.

These results could be used to find the means of controlling or at least reducing pollutions of the atmosphere and the oceans where stratified flows prevail.

Progress During FY 1996:

During this period, Professor Chigier and his students have continued fine-tuning of the TSI two-axis LDV system. The new system allows making measurements in coincidence mode with a coincidence window of 0.5 ms. The net data rate in this mode is on the order of 100 Hz. Flow seeding has been greatly improved. The TSI six-jet atomizer continues to generate liquid droplets for seeding the flow in the tunnel.

In summary, the low speed stratified shear layer wind tunnel has been built and shown to meet all of the performance criteria required for the experiments objectives. LDV measurements of an unstratified shear layer were made as a baseline for comparison.

LDV measurements in both stably and unstably stratified shear layers have also been made. As expected, the axial mean velocity profiles do not show significant dependence on sign of the density gradient beyond the translation of the whole flow. The vertical velocity profile at the nozzle exit shows great dependence on the existence of a density gradient. The downstream vertical velocity profiles do show dependence on the sign of the density gradient. For the unstably stratified case, the ascent of the mixing layer is less than the vertical velocity is more nearly uniform across the layer.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/93 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-24-05-71

NASA CONTRACT NO.: NAG3-150

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Chigier, N. and Humphrey, W., "Transport phenomena in stratified multi-fluid flow in the presence and absence of gravity." Third Microgravity Fluid Physics Conference, 1996.

Bubble Dynamics, Two-Phase Flow, and Boiling Heat Transfer in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Jacob N. Chung

Washington State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The main objective is to study the effects of external force fields on the nucleation, two-phase bubble dynamics and boiling transport in microgravity. The proposed research seeks to increase our understanding of bubble nucleation and growth on the heater surface, bubble removal from the heater surface by an electric field, an acoustic field or a velocity shear resulting from the relative fluid motion with respect to the surface, and bubble dynamics and heat and mass transport in boiling liquids.

Task Description:

In the experimental portion, visualizations with NTSC and high-speed photography of the boiling process and heat transfer measurements have been performed in a drop tower at Washington State University. The visualization photographs were then analyzed by a digital image analysis system. Boiling curves were developed based on measurements of heat fluxes and surface superheats for various system conditions. Special attention was focused on the critical heat flux. Analytical and numerical modeling is also included to compliment the experiments. Perturbation and asymptotic techniques will be applied for low Reynolds number bubble dynamics, linearized bubble stability analysis, and small oscillation of bubble in microgravity to account for small disturbances and the g-jitter.

Task Significance:

The proposed research seeks to:

1. Increase our understanding of bubble nucleation and growth on the heater surface.
2. Bubble removal from the heater surface by an electric field, an acoustic field, and velocity shear resulting from the relative fluid motion with respect to the surface.
3. Bubble dynamics and heat and mass transport in boiling liquids.

Future spacecraft power systems are likely to have greater power generation and dissipation requirements due to proposed longer space missions and more intensive space activities. Without suffering from weight penalties, two-phase boiling systems are being considered for a wide range of future space applications such as thermal control, propulsion, power generation, and thermal management. The boiling system has the potential advantage of being able to transfer a large amount of energy over a relatively narrow temperature range with small weight requirements. For example, two-phase systems were once baselined for the space station. However, the thermo-fluid dynamics of two-phase systems in microgravity encompasses a wide range of complex phenomena that were not understood sufficiently for the engineering design to proceed.

Progress During FY 1996:

We have made substantial progress in the following four areas:

1. Facilities:

The 2.1 Second Drop Tower is working well and over 250 drops have been completed. The drop tower construction and calibration results, including air bag design and residual acceleration results have been published. We have also completed the conversion of our 0.6 second air bag Drop Tower into a 1.2 Second Drop Tower. We have changed from plastic to glass in our heater design with very successful results. One of these heaters has lasted for over thirty drops with heat fluxes up to 8 W/cm^2 . Our single bubble heaters are also now sputtered on glass and can generate hundreds of individual bubbles before any noticeable degrading effects on the heater.

2. Acoustic Driven Nucleate Boiling:

The purpose of the acoustic driven boiling research is to determine if an acoustic sound field can maintain nucleate pool boiling in microgravity and measure its effects on the boiling process in microgravity and terrestrial gravity. This research is complete and has been written up as a MS thesis. The application of the acoustic sound field to the boiling process increases the heat transfer rates in Earth's gravity. In microgravity it was found that the radiation pressure can produce a large enough acoustic force to move vapor bubbles off a heater surface during microgravity. The effects of cavitation and acoustic streaming resulted in erratic bubble motion and aided in the perturbation of vapor bubbles attached to and in the vicinity of the heater and effected the heat transfer and bubble dynamics in both microgravity and terrestrial gravity. At all heat fluxes tested during microgravity, the acoustic mechanisms prevented large amounts of vapor from blanketing the heater surface.

3. Forced-Convection Nucleate Boiling:

The purpose of the forced-convection boiling research is to determine if a flow field can maintain nucleate pool boiling in microgravity and measure its effects on the boiling process in both microgravity and terrestrial gravity. We presented a paper on the work of Wang et al. 1993 at the National Convective Boiling Conference in Banff, Canada. The paper received favorable reviews and, as a result, it will be published in a new book entitled "Convective-Flow Boiling". In continuation of this work, we are presently utilizing a small flow boiling rig in the 1.2 Second Drop Tower and have completed over 40 drops with both 1" x 1" gold film heaters and with single bubble heaters. The continued research will attempt to map the boiling regimes for various flow rates and heat fluxes in microgravity. For example, at a given heat flux, what flow rate is required in order to sustain boiling and avoid burnout of the heater surface.

4. Electrostatic Driven Nucleate Boiling:

The purpose of the electrostatic boiling research is to determine if an electric field can maintain nucleate pool boiling in microgravity and measure its effects on the boiling process in both microgravity and terrestrial gravity. We have studied how large nonuniformities in the electric field produced at the edge of two diverging-plate electrodes can produce large forces which are efficient in motion control and bubble positioning for both liquid droplets and vapor bubbles. Three electric-field experimental studies are either completed or under progress. The first study focuses on results in which a controlled electrical body force is imposed onto the boiling process for a test fluid of FC-72 which is boiled on a horizontal platinum wire heater. As this force tends to either add to or subtract from buoyancy an analogy between variable gravity boiling results and results from boiling with an electric field are presented and discussed. Second, an experiment was performed to correct some mistakes previously reported in the literature. We have published a paper in the J. of Applied Physics detailing this information. The third and final set of experiments uses semitransparent gold-film heaters which allow a bottom view of the boiling. We are also using a special surface that changes color with temperature and allows us to visualize how the temperature varies over the heater surface.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	1
PhD Students:	1	PhD Degrees:	0

TASK INITIATION: 12/92 EXPIRATION: 8/97

PROJECT IDENTIFICATION: 962-24-05-59

NASA CONTRACT NO.: NAG3-138

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Snyder, T.J. and Chung, J.N., Residual acceleration as a function of frequency for a 2.1 second drop tower with a "drag shield" design. International J. of Microgravity Science & Technology, vol. VIII, pp. 261-264 (December 1995).

Snyder, T.J., Schneider, J.B., and Chung, J.N., A second look at electrokinetic phenomena in boiling. J. Applied Physics, vol. 79, pp. 6755-6760 (1996).

Wang, T.C., Snyder, T.J., and Chung, J.N., Experimental examination of forced-convection subcooled nucleate boiling and its application in microgravity. ASME J. Heat Transfer, vol. 118, pp. 237-241 (February 1996).

Proceedings

Chung, J.N., Snyder, T.J., and Sitter, J.S., "Microgravity boiling in an external force field." Proceedings of the 20th International Symposium on Space Technology and Science, held in Gifu, Japan, pp. 195-200, May 19-25, 1996.

Snyder, T.J., Chung, J.N., and Schneider, J.B., "A study on the competing effects of the dielectrophoretic force and buoyancy on nucleate boiling heat transfer rates and on analogy with variable gravity boiling results." Proceedings of the ASME International Mechanical Engineering Conference, Atlanta, GA, November 17-22, 1996.

Presentations

Snyder, T.J., "Studies on the dielectrophoretic force and its effects on boiling bubble dynamics and heat transfer in terrestrial and microgravity environments." Washington State University, December 1995.

Microgravity Particle Dynamics

PRINCIPAL INVESTIGATOR: Dr. Ivan O. Clark

NASA Langley Research Center (LaRC)

Co-INVESTIGATORS:

Johnson, E.J.
Meyers, J.F.
Kjelgaard, S.O.

Lockheed Engineering & Sciences Co.
NASA LaRC/RTG/FldMD/NDB
NASA LaRC/RTG/FldMD/EMB

Task Objective:

The objective of this research was to develop the apparatus, numerical models, and practices for enhancing the knowledge of particle transport in laminar fluid flows. Specifically, an enhanced understanding of the roles of thermophoresis (thermal gradient) and Saffman (particle crossing of velocity gradient) effects on particle transport was sought while investigating the critical parameters and instrumentation requirements for subsequent microgravity experiments.

Task Description:

The technical approach was a coordinated numerical and experimental investigation using geometries selected to maximize the scientific return of the research. Gravitational effects in the experimental investigation were addressed through the use of multiple orientations, relative to gravity, of the test chambers. The first step in this investigation was a parametric study to determine the order of magnitude of the competing effects for candidate test chamber geometries. These complex interacting effects included gravity, buoyancy, inertia, viscous drag, particle rotation, electrostatic charges, as well as thermal and velocity gradients.

Task Significance:

The research attempted to develop: (1) definition of the requirements and the potential for follow-on flight experiments in transport phenomena, (2) an enhanced understanding of particle transport phenomena in thermal and velocity gradients, and (3) fluid dynamic correction factors for particle-based flow instrumentation for a range of thermophoresis and Saffman environments. The results of this research will be immediately applicable in both unigravity and microgravity for applications such as validation of particle transport theories; correction of wind tunnel research data; and design refinements for chemical vapor deposition reactors, particulate combustors, and clean rooms. In addition, experimental size constraints for microgravity experiments dictate that velocity gradients will exist in laminar flow flight experiments. Hence, Saffman effects will be present to some extent in all microgravity laminar flow experiments with particles.

Progress During FY 1996:

Parametric studies of velocity, length, time, thermal gradient magnitude and velocity gradient magnitude likely to be involved in gas-solid multiphase flight experiments have been assessed for 1-100 micrometer particles. The results of this parametric study indicate that flight experiment regimes are both achievable and useful. Validation testing of a version of FLUENT augmented to analyze particle nucleation and growth during transport was initiated. Comparison of parametric study predictions with laser velocimetry and infrared imaging results were begun.

A database has been established of particle dynamics research and particle-based instrumentation which will ensure currency of ground and flight experiments associated with this research as well as provide a valuable reference tool for other researchers in this area.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 11/92 **EXPIRATION:** 11/95

PROJECT IDENTIFICATION: 962-24-06-04

RESPONSIBLE CENTER: LaRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Johnson, E.J., Hyer, P.V., Culotta, P.W., and I.O. Clark, I.O. Evaluation of infrared thermography as a diagnostic tool in CVD applications. *J. Crystal Growth*, submitted, (1996).

Presentations

Clark, I.O. "Characterization of flows in a horizontal CVD system using laser velocimetry and thermal imaging." Tenth American Conference on Crystal Growth, Vail, CO, August 4-9, 1996.

Clark, I.O. and Johnson, E.J. "Microgravity particle dynamics." Third Microgravity Fluid Physics Conference, Cleveland, OH, June 13-15, 1996.

Humphries, Jr., W.M, Bartram, S.M., and Clark, I.O. "Velocity field measurements in a chemical vapor deposition reactor using digital particle image velocimetry." 1996 ASME Symp Laser Anemometry and Experimental and Numerical Flow Visualization, San Diego, CA, July 7-11, 1996.

Structure, Shape Instabilities, and Phase Transitions of Freely Suspended Liquid Crystal Bubbles

PRINCIPAL INVESTIGATOR: Prof. Noel A. Clark

University of Colorado, Boulder

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The experimental study of smectic liquid crystal films in the form of single levitated bubbles including studies of (1) dynamic and equilibrium in-plane stress-induced shapes of levitated bubbles, (2) stress-induced quenches of the Kosterlitz-Thouless phase transition among others, and (3) studies of film permeability.

Task Description:

These experimental studies require technique developments beyond those which have been used for the study of planar films in 1g. Among the more important ones are (1) a method for inflation, levitation, positional stabilization, of the bubble, (2) transmission video microscopy to monitor bubble shape and polarized reflection video microscopy to probe the local orientation, and (3) methods to change ambient gas pressure while maintaining bubble position.

Task Significance:

This study is suitable for several novel lines of experimentation of relevance to the physics of both liquid crystals and fluid thin films. These ultra thin freely suspended liquid crystal films are structures of fundamental interest in condensed matter physics. They are the thinnest known stable condensed phase preparation, making them ideal for studies of two dimensional phase transitions and of fluctuation and interface phenomena of thin fluid films. Freely suspended films have been used to provide unique experimental conditions for the study of condensed phase transitions on two dimensions.

Progress During FY 1996:

The inherent fluid-layer structure and low vapor pressure of smectic liquid crystals enable the long term stabilization of freely suspended, single component, liquid crystal films as thin as 30 Å, a single molecular layer. These structures have been intensively studied as planar films freely suspended over holes in solid substrates, experiments which have been crucial to the current understanding of liquid crystal phase behavior.

In this project the study of these smectic liquid crystal films in the form of bubbles was emphasized. This bubble geometry makes accessible a variety of important new experiments.

• **Quenching the Smectic A to C Transition**

During the quick deflation of a smectic C (////////) bubble, there is in-plane compression which forces the tilted smectic C molecules to stand up, giving transient formation of smectic A (||||||). When the deflation completes the smectic C returns but the field giving the tilt direction in the layer plane is full of topological defects. These defects can be observed on the film by polarized reflection microscopy. This system is a two dimensional analog of the symmetry breaking phase transition corresponding to the appearance of matter in the early universe. A scaling model has been developed along with a computer simulation of the process which explains the time behavior. The films have enabled the precise determination of smectic layer electron density and positional fluctuation profile, and have been used to show that the interlayer interactions in antiferroelectric tilted smectics are strictly nearest neighbors.

• **Permeation of Helium through Ultrathin Organic Films**

Bubble photos have shown typical 2cm diameter bubbles with thick regions (approx. 15 layers) and thin regions (approx. 5 layers). Such a bubble, if filled with helium, will completely deflate via permeation of helium through the thin region in about 10 seconds. The permeation rate of helium through the film can be measured using this deflation rate. Currently, optical reflectivity is being used as a measure of film thickness.

• Annealing of a Two Dimensional Foam

In other bubble photos the thick regions are large and contiguous. After aggressive shearing of the bubble by an air jet the thicker region forms a foam of very small pancake-like circular islands, which slowly coalesce and coarsen and settle by gravity to the bottom. The coarsening dynamics of this novel 2 dimensional system are presently being studied.

In pursuing the goal of an eventual microgravity experiment, a variety of techniques for generating and stabilizing bubbles has been developed. Preliminary experiments have begun on a novel system of coalescing droplets in two dimensions. Also developed were theoretical models for the nonequilibrium behavior of topological defect arrays generated by the in-plane compressional quenching through the 2D XY order-disorder (Kosterlitz-Thouless) transition in smectic C bubbles.

The Principal Investigator and his team are now in a position to measure coefficients of simple gases through freely suspended liquid crystal films via atomistic molecular dynamics and Monte Carlo computer simulation. During the past several years, a variety of effective computational tools have been developed for the simulation of realistic liquid crystal models, including the development of an improved empirical force field specifically designed for modeling liquid crystalline materials and the development of special simulation techniques enabling efficient configuration-space and conformational sampling in realistic liquid crystal simulations. This methodology has been used in the study of a variety of systems, ranging from simulations of single molecules in a mean-field orientational potential, to large-scale, many-molecule simulations of systems containing as many as 108 molecules. These latter studies include the first reported simulation studies of freely suspended smectic films with full atomic detail. Additional work in these areas will be forthcoming in a follow-on grant (addressing bubble and tube geometries) which has already been awarded.

Work on this grant has been completed and requirements fulfilled as of May 1996.

STUDENTS FUNDED UNDER RESEARCH:				TASK INITIATION: 4/94		EXPIRATION: 3/96	
BS Students:	0	BS Degrees:	0	PROJECT IDENTIFICATION: 962-24-05-82			
MS Students:	0	MS Degrees:	0	NASA CONTRACT NO.: NAG3-160			
PhD Students:	2	PhD Degrees:	1	RESPONSIBLE CENTER: LeRC			

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Ginzburg, V.V., Beale, P.D., and Clark, N.A., Scaling analysis of particle annihilation systems with long range interaction. Physical Review Letters, (accepted 1996).

Muzny, C.D., Clark, N.A., and Gun Won J., Quenching the Kosterlitz-Thouless transition in two dimensional freely suspended liquid crystal films. Physical Review Letters, (accepted 1996).

Pang, J. and Clark, N.A., Dynamics of layer steps in freely suspended liquid crystal films. Bulletin of the American Physical Society, 40,85 (October 1995).

Structure, Hydrodynamics, and Phase Transitions of Freely Suspended Liquid Crystals

PRINCIPAL INVESTIGATOR: Prof. Noel A. Clark

University of Colorado, Boulder

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The purpose of the proposed research is to develop those aspects of the physics of freely suspended liquid crystal films for which the microgravity environment would be necessary and useful.

The proposed research will develop techniques that will enable the novel study of freely suspended liquid crystals and films in microgravity. This series of experiments have the following objectives:

- Study the shape of bubbles having a layer structure that is isotropic two-dimensional liquid under conditions of changing in-plane stress, i.e. probe whether the surface tension of a fluid film in air can be reduced to zero.
- Compressionally induce the smectic A to smectic C transition in order to understand what happens when a Kosterlitz-Thouless system is quenched and to probe the coarsening dynamics of a simple vortex annihilation process.
- Study the coupling of in-plane structure to bubble or tube shape.
- Study of the gas permeability of mono- and multi-layer liquid films: Experiments and computer simulations.
- Generation and coalescence of two dimensional foams of islands on a bubble surface.
- Develop techniques for inflating bubbles and tubes under conditions that the number of layers and bubble size can be controlled.
- Develop techniques for detaching and levitating bubbles in a 1G environment.
- Develop observational and measuring techniques for the physical quantities of interest.
- Develop techniques for changing and controlling chamber pressure.
- Study the shape of bubbles under conditions of static and dynamic in-plane stress and/or in-plane anisotropy.
- Study compressionally induced in-phase transitions.
- Study of the gas permeability of few layer thick liquid films.

Task Description:

The proposed experiments allow the study of smectic liquid crystal films in nonplanar geometries, in the form of bubbles and tubes. These geometries will make accessible a variety of important new experiments not possible in planar films, reducing the film edge to area ratio and enabling the study of the coupling of curvature to in-plane structure. The research proposed includes: Study of the coalescence dynamics of two-dimensional foams of islands on the surface of a bubble; investigation of dynamic and equilibrium in-plane stress-induced shapes of bubbles, including those with anisotropic in-plane order; stress-induced quenches of the Kosterlitz-Thouless phase transition and other in-plane two-dimensional phase transitions; and studies of film permeability. These experiments will require technique developments beyond those which have been used for the study of planar films including: Methods for the inflation, levitation, and positional stabilization of smectic liquid crystal bubbles and tubes at 1G; transmission video microscopy to monitor bubble shape and polarized reflection video microscopy to probe the

local molecular orientation field and island distribution; methods to change ambient gas pressure while fixing bubble position; and simulation techniques for calculating film permeability and stability.

Task Significance:

These ultrathin freely suspended liquid crystal films are structures of fundamental interest in condensed matter physics. They are the thinnest known stable condensed phase structures and have the largest surface-to-volume ratio of any condensed phase preparation, making them ideal for studies of two dimensional phase transitions and of fluctuation and interface phenomena of thin fluid films. Freely suspended films have been a wellspring of new liquid crystal physics. They have been used to provide unique experimental conditions for the study of condensed phase transitions in two dimensions. They are the only system in which the hexatic has unambiguously been identified as a phase of matter, and the only physical system in which fluctuations of a 2d XY system and Kosterlitz-Thouless phase transition has been visualized and 2d XY quasi long range order observed. The films have enabled the precise determination of smectic layer electron density and positional fluctuation profile and have been used to show that the interlayer interactions in antiferroelectric tilted smectics are strictly nearest neighbors.

Progress During FY 1996:

This is a new grant which was awarded on May 2, 1996. Graduate student hiring has been completed, and equipment has been ordered. Assembly of hardware/equipment is currently underway.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NAG3-184

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Glaser, M.A. and Clark, N.A., Statistics of local order in two dimensional liquids: The geometrical defect condensate controls the statistics of local order in a two dimensional liquid. Science, (1995).

Glaser, M.A., Malzbender, R., Clark, N.A. and Walba, D.M., Atomic-detail simulation studies of smectic liquid crystals. Molecular Simulation, (1995).

Fluid Interface Behavior Under Low- and Zero-Gravity Conditions

PRINCIPAL INVESTIGATOR: Prof. Paul Concus

University of California, Berkeley

CO-INVESTIGATORS:

Finn, R.

Stanford University

Task Objective:

The general objective of this research is to gain better mathematical understanding of the physical behavior of fluids partly filling a container or otherwise in contact with solid support surfaces when capillary forces predominate. Closely interrelated with the mathematical and computational studies are current and planned ground-based and in-space microgravity experiments.

Task Description:

The approach for this project is to pursue parallel theoretical, computational, and experimental studies to explore equilibrium capillary free surface interfaces in a variety of geometrical configurations. The theoretical aspects include both rigorous mathematical studies and numerical computation. The experimental aspects are carried out in collaboration with M. Weislogel of NASA Lewis Research Center; these include current and proposed space experiments in the glovebox facilities on the NASA Space Shuttle and the Russian *Mir* Space Station. Of particular interest are configurations for which small changes in container shape or contact angle can give rise to large bulk reorientation of fluid.

Task Significance:

Knowledge gained from these studies can lead to a better understanding of surface phenomena of liquids in containers under low-gravity and, in particular, to obtaining new information on the significance of contact angle as an intrinsic physical property. Additionally, development of accurate, new methods for measuring contact angle and new insights for managing fluids in space can result.

Progress During FY 1996:

Work continued on studying a class of "canonical proboscis" containers. These containers are cylinders whose sections have the remarkable property that at a prescribed contact angle a "nearly-discontinuous" transition of bulk fluid occurs, with unbounded rise height over a "proboscis" protrusion; the protrusion can be made relatively as large as desired. The proboscis containers, as well as a movable wedge container, comprise a glovebox experiment carried out on the USML-2 flight this year. These shapes have possible application to exploiting microgravity for the accurate determination of contact angle; in this regard, double proboscis containers were designed for the experiment, to permit bracketing of the determined contact-angle values. Video-tape data from the experiment is currently being analyzed.

Investigation continued of a new type of discontinuous behavior, inferred from contrasting results of a student L. Zhou on liquid bridges between parallel plates and of a student J. McCuan on nonexistence of tubular bridges in wedge domains. As a consequence of their results, we have shown that regardless of the stability criteria for a liquid drop trapped between parallel plates, such drops are in general unstable with respect to tilting of one of the plates. Fairly precise information can be given as to the kinds of discontinuous behavior to be expected. The Angular Liquid Bridge glovebox experiment based on this work has been developed, jointly with M. Weislogel, and is scheduled for the *Mir* 23/NASA 4 mission in FY 1997.

A separate glovebox experiment is currently being flown on the *Mir* 21/NASA 2 mission. This experiment is a continuation our USML-1 investigation, which concerns axially symmetric "exotic" containers. The containers, which are in the shape of a right circular cylinder with mathematically derived toroidal-like bulge, have the property that they admit in zero gravity an entire continuum of axially symmetric equilibrium interfaces for the prescribed fluid volume and contact angle. However, it was proved that the entire container can admit no symmetric stable interface; thus the energy minimizing interface (which is known to exist) must necessarily be asymmetric. This behavior was verified in the USML-1 experiment. As the fluid enters the bulge in the container, it appears at first as a spherical cap; but in response to a disturbance it immediately adopts an asymmetric shape. In the present *Mir*

experiment an attempt is made to obtain other equilibria, predicted numerically, and to examine their stability.

Work continued on studying the behavior of capillary surfaces in wedge domains, in which the contact angles on the two sides of the wedge are allowed to differ. We showed earlier that if the values of contact angle satisfy certain relationships, then a surface satisfying the equilibrium equations for zero gravity must have discontinuous unit normal at the vertex. The existence of such surfaces in particular configurations has now been proved. Furthermore, as part of a work in progress with J.T. Chen and E. Miersemann, it has been shown that, despite the singularity in the surface normal, the solution height must be *a priori* bounded above and below at the vertex. Additionally, it has been proved that not only the normal vectors but also the solution heights themselves are discontinuous at the vertex. This last result is in accordance with numerical calculations by H. Mittelman indicating that the discontinuity can become vanishingly small near the sides of the rectangle, but is nevertheless present. It would be of interest to determine what actually happens in physical experimental situations.

In new joint work with J. McCuan, it has been proved that if a fluid drop in zero gravity lies in the edge of a wedge-shaped domain formed by two planes intersecting in angle 2α , and if the contact angle γ is such that $|\pi - 2\gamma| \leq 2\alpha < \pi$, then the surface of the drop must be spherical. If the first of those inequalities is reversed, the fluid will flow out to infinity along the edge; if the second is reversed, calculations suggest that the fluid configuration will be unstable. A consequence of the result is that for prescribed volume there is exactly one such drop, thus identifying another of the very few configurations for which uniqueness of capillary surfaces is known. (In general, non-uniqueness has to be expected.) It is conjectured that the same result holds for a trihedral angle, and under some conditions that result has been proved. It is shown that if more than three edges cut through the drop's surface, then the surface need not be spherical. The results suggest new microgravity experiments, on the behavior of a drop situated in a tetrahedral container and with steadily increasing volume; remarkable and unexpected behavior can be anticipated, depending on the particular geometries and contact angles, and the initial (small volume) configuration.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 3/90 EXPIRATION: 3/96

PROJECT IDENTIFICATION: 962-24-05-66

NASA CONTRACT No.: NCC3-329

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Chen, A., Concus, P., Finn, R., and Weislogel, M., On cylindrical container sections for a capillary free-surface experiment. Lawrence Berkeley Lab, Report LBL-36629 Rev., (Nov. 1995).

Concus, P. and Finn, R., Comments on a paper by Keller, King, and Merchant. Nonlinear Anal., (1996).

Concus, P. and Finn, R., Capillary wedges revisited. SIAM J. Math. Anal., 27, pp. 56-69 (1996).

Finn, R., Local and global existence criteria for capillary surfaces in wedge domains. Calculus of Variations, 4, pp. 305-322 (1996).

Finn, R., On a proposition of Lancaster and Siegel. Mathematics Institute, University of Leipzig, (1996).

Finn, R. and Marek J.M., The modified canonical proboscis. Zeit. Anal. Anwend., 15, pp. 95-108 (1996).

McCuan, J., Symmetry by spherical reflection and spanning drops in a wedge. Pacific J. Math, (in press, 1996).

Zhou, L.-M., On stability of a catenoidal liquid bridge. Pacific J. Math., (in press, 1996).

NASA Tech Briefs

Concus, P., Finn, R., Weislogel, M.M., Interface Configuration Experiments (ICE) Explore the Effects of Microgravity Fluids," Research and Technology (R and T) , . NASA Tech Brief, NASA TM 107111, pg 140 (October, 1995).

Proceedings

Concus, P. and Finn, R., "Equilibrium free-surface configurations: mathematical theory and space experiments." 27th AIAA Fluid Dynamics Conference, New Orleans, Paper AIAA 96-2047, June 1996.

Concus, P., Finn, R., and Weislogel, M., "Proboscis container shapes for the USML-2 ." Interface Configuration Experiment, in Materials and Fluids Under Low Gravity, L. Ratke, H. Walter, and B. Feuerbacher, eds., Lecture Notes in Physics Vol. 464, Springer-Verlag, Berlin, 1996, pp. 261–270.

Finn, R., "On solutions of mean curvature type inequalities, in Partial Differential Equations and their Applications." P. Marcellini, G. Talenti, and E. Vesentini, eds., Marcel Dekker, pp. 147–154, 1996.

Presentations

Concus, P. and Finn, R., "Equilibrium Fluid Interface Behavior Under Low- and Zero-Gravity Conditions." Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 13-15, 1996.

Finn, R., "Capillary surfaces in wedge domains: new results." World Congress of Nonlinear Analysts, Athens, Greece, July 1996, and Univ. Dresden, Germany, June 1996.

Finn, R., "Capillary surfaces, theory and experiment, from kitchen sink to NASA Space Shuttle." Univ. Leipzig, Germany, June 1996, and Sonoma State Univ., April 1996.

Finn, R., "Regularity properties of capillary surfaces." Univ. Bochum, Germany, May 1996.

Fluid Interface Behavior Under Low- and Zero-Gravity Conditions

PRINCIPAL INVESTIGATOR: Prof. Paul Concus

University of California, Berkeley

CO-INVESTIGATORS:

Finn, R.

Stanford University

Task Objective:

The general objective of this research is to gain better mathematical understanding of the physical behavior of fluids partly filling a container or otherwise in contact with solid support surfaces when capillary forces predominate. Closely interrelated with the mathematical and computational studies are current and planned ground-based and in-space microgravity experiments.

Task Description:

The approach for this project is to pursue parallel theoretical, computational, and experimental studies to explore equilibrium capillary free surface interfaces in a variety of geometrical configurations. The theoretical aspects include both rigorous mathematical studies and numerical computation. The experimental aspects are to be carried out in collaboration with M. Weislogel of NASA Lewis Research Center; these include currently scheduled and proposed space experiments in the glovebox facilities on the Russian *Mir* Space Station and NASA Space Shuttle. Of particular interest are configurations for which small changes in container geometry or contact angle can give rise to large bulk reorientation of fluid.

Task Significance:

Knowledge gained from these studies can lead to a better understanding of surface phenomena of liquids in containers under low-gravity and, in particular, to obtaining new information on the significance of contact angle as an intrinsic physical property. Additionally, development of accurate, new methods for measuring contact angle and new insights for managing fluids in space can result.

Progress During FY 1996:

This project is an outgrowth of our current Task NCC3-329, soon to expire, which is reported separately. The project has not been initiated yet, but shall be once funding has been established, probably at the end of FY 1996 or at the beginning of FY 1997. Our initial focus will be on studies related to the scheduled *Mir* 23/NASA 4 Angular Liquid Bridge glovebox experiment and on continuation of the other topics described under Task NCC3-329.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 1

TASK INITIATION: 8/96 EXPIRATION: 8/98

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NAG3-194

RESPONSIBLE CENTER: LeRC

Interface Morphology During Crystal Growth: Effects of Anisotropy and Fluid Flow

PRINCIPAL INVESTIGATOR: Dr. Sam R. Coriell

National Institute of Standards and Technology

CO-INVESTIGATORS:

McFadden, G.B.

National Institute of Standards and Technology

Murray, B.T.

National Institute of Standards and Technology

Manning, J.R.

National Institute of Standards and Technology

Task Objective:

During the directional solidification of a binary alloy solute inhomogeneities can arise from both fluid flow and morphological instability. In microgravity buoyancy-driven fluid flow is reduced, and experiments to study the evolution of morphological patterns without the interference of fluid flow may be possible. Another goal is to develop an understanding of the interaction of fluid flow with the crystal-melt interface so that solute segregation in solidifying alloys can be controlled in order to obtain materials with superior properties on Earth as well as in a microgravity environment.

Task Description:

This research consists of theoretical studies of the interaction of fluid flow with the crystal-melt interface. When growth is by step motion, kinetic anisotropy provides enhanced morphological stability. Shear flows along the interface interact strongly with the step motion and cause decreased stability for a flow in the same direction as the step motion and enhanced stability for flows counter to step motion. We plan to investigate these flow-interface interactions for a wide range of processing conditions for melt and solution growth with extension to more complex physical models and nonlinear interface morphologies. Calculations of solute segregation and interface stability for specific alloys and processing conditions relevant to past and future space experiments will also be performed.

Specific research tasks include:

Linear and non-linear stability calculations treating highly anisotropic kinetics due to growth by step motion.

Linear stability analyses of the interaction of fluid flow with the crystal-melt interface for growth from supersaturated solutions.

Generalization of the standard morphological stability theory in order to allow a critical comparison with experimental measurements in space experiments.

Numerical calculations relevant to previous and planned space experiments on interface stability, including the effect of g-jitter on fluid flow and solute segregation.

Task Significance:

Solute segregation during alloy solidification and crystal growth determines the properties of the solidified material. The length scale associated with the spatial distribution of solute (microsegregation) is established by the morphology of the crystal-melt interface (cellular or dendritic). Fluid flow in the liquid results in macrosegregation of solute. This research will determine the processing conditions required to eliminate microsegregation and produce alloys with desirable microstructures and improved properties.

Progress During FY 1996:

In collaboration with A. A. Chernov, the effect of a parallel shear flow and anisotropic interface kinetics on the onset of (linear) instability during growth from a supersaturated solution was analyzed including perturbations in the flow velocity. The model used for anisotropy is based on the microscopic picture of step motion. A shear flow (linear Couette flow or asymptotic suction profile) parallel to the crystal-solution interface in the same direction as the step motion (negative shear) decreases interface stability. For large wave numbers k_x , the perturbed flow field can be neglected and a simple analytic approximation for the stability-instability demarcation is found. A shear

flow counter to the step motion (positive shear) enhances stability and for sufficiently large shear rates (on the order of $1/s$) the interface is morphologically stable. Alternatively, the approximate analysis predicts that the system is unstable if the solution flow velocity in the direction of the step motion at a distance $1/2 k_x$ from the interface exceeds the propagation rate v_x of step bunches induced by the interface perturbations. The approximate results are applied to the growth of Ammonium Dihydrogen Phosphate (ADP) and protein crystal. For sufficiently low super-saturations, the interface is stable for positive shear and unstable for negative shear. More generally, there is a critical negative shear rate for which the interface becomes unstable as the magnitude of the shear rate increases. For a range of growth conditions for ADP, the magnitude of this critical shear rate is $2 k_x v_x$. Even shear rates due to natural convection may be sufficient to affect stability for typical growth conditions.

In collaboration with R. F. Sekerka, we have used a stagnant film model of the effect of natural convection on the dendrite operating state (tip radius and velocity) and have studied possible effects of the container size used in the microgravity experiments of Glicksman et al. We find that the thickness of boundary layer thickness of the stagnant boundary layer thickness is always much larger than the tip radius. In Earth's gravity, the boundary layer thickness is always much smaller than the characteristic size of the container, but in microgravity, the boundary layer thickness is comparable to the character container size. A model in which the boundary layer thickness is about 1 cm fits the microgravity data for the dendrite tip radius and velocity as a function of supercooling about as well as one in which the value of the boundary layer thickness is based on natural convection in an infinite container.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: C-31002E

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Coriell, S.R., Murray, B.T., Chernov, A.A., and McFadden, G.B., Effects of shear flow and anisotropic kinetics on the morphological stability of a binary alloy. *Metallurgical and Materials Trans.*, 27A, pp. 687-694 (1996).

Favier, J.J., Lehmann, P., Drevet, B., Garandet, J.P., Camel, D. and Coriell, S.R., A study of morphological stability during directional solidification of a Sn-Bi alloy in microgravity, in materials and fluids under low gravity. *Lecture Notes in Physics*, ed. L. Ratke, H. Walter, and B. Feuerbacher (Springer-Verlag, Berlin), vol. 464, p. 77-94 (1996).

Sekerka, R.F., Coriell, S.R., and McFadden, G.B., Stagnant film model of the effect of natural convection on the dendrite operating state. *J. Crystal Growth*, 154, pp. 370-376 (October 1995).

Warren, J. A. and Murray, B. T., Ostwald ripening and coalescence of a binary alloy in two dimensions using a phase-field model. *Modelling Simul. Mater. Sci. Eng.*, 4, pp. 215-229 (1996).

Wheeler, A.A., McFadden, G.B., and Boettinger, W.J., Phase-field model for solidification of a eutectic alloy. *Proc. R. Soc. Lond. A*, 452, pp. 495-525 (1996).

Presentations

Coriell, S. R., Murray, B. T., Chernov, A. A., and McFadden, G. B., "Step bunching on vicinal stepped faces growing from solutions and melts." Tenth American Conference on Crystal Growth, Vail, CO., August 1996.

Coriell, S.R., Murray, B.T., Chernov, A.A., and McFadden, G.B., "The effect of a shear flow on the morphological stability of a vicinal face: growth from a supersaturated solution." 31st COSPAR Scientific Assembly, Birmingham, England, July 1996.

Murray, B.T., "The phase-field equations as a computational technique in crystal growth." Tenth American Conference on Crystal Growth, Vail, CO., August 1996.

Phoretic and Radiometric Force Measurements on Microparticles under Microgravity Conditions

PRINCIPAL INVESTIGATOR: Dr. E. J. Davis

University of Washington

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

- (a) Develop and improve techniques and apparatus for precise measurement of phoretic and radiometric forces.
- (b) Measure phoretic forces over a range of Knudsen numbers in the transition regime to validate existing theories for spherical particles and determine accommodation coefficients for energy, mass and momentum.
- (c) Determine the effects of particle morphology (irregular shape), gas properties and particle properties on phoretic forces.
- (d) Explore the effects of natural convection on phoretic force measurements in the near-continuum regime to determine the conditions, parameters and system properties which can only be studied reliably under microgravity conditions. Measurements at reduced pressures can be carried out via ground-based experiments.
- (e) Develop lower weight and more compact instrumentation for the measurement of phoretic forces under microgravity conditions in space flight.

Task Description:

The proposed four year program involves ground-based measurements using electrodynamic balances, which simulate zero-gravity conditions by trapping the particle with electric fields and design studies of apparatus suitable for space flight. At atmospheric pressure it is difficult to eliminate convection in the gas phase in such ground-based experiments when the required temperature and/or concentration gradients are imposed on a particle. The laboratory studies will provide information on the parameters which need to be measured and controlled in microgravity experiments and will lead to the design of apparatus suitable for phoretic force measurements under microgravity conditions.

Task Significance:

This experimental and analytical research program is proposed to investigate phoretic and radiometric forces on particles and droplets (submicrometer and micrometer sizes) in a gaseous environment. Under microgravity conditions such forces become the dominant force on a microparticle, so measurements made under microgravity conditions represent a unique way to study the basic fluid physics of the transport of heat, mass and momentum between a gas and solid or liquid particulate matter.

Of specific interest is the determination of mass, momentum and energy accommodation coefficients, which are needed for the prediction of phoretic forces in the noncontinuum regime. Measurements made under the influence of normal gravity are affected by convection, which obscures the forces of interest. Applications of these forces arise in numerous technologies, including combustion, electronic water decontamination, fiber optic production, nuclear reactor decontamination, containerless processing and particle deposition processes.

Progress During FY 1996:

This is a new grant which was awarded in May 1996. Graduate students have been hired, and equipment has been ordered. Hardware assembly is currently underway.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 5/96 EXPIRATION: 4/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-183

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Li, W. and Davis, E.J., The effects of gas and particle properties on thermophoresis. J. Aerosol Sci, (1995).

Interaction and Aggregation of Colloidal Biological Particles and Droplets in Electrically-Driven Flows

PRINCIPAL INVESTIGATOR: Prof. Robert H. Davis

University of Colorado, Boulder

CO-INVESTIGATORS:

Todd, P.
Loewenberg, M.

University of Colorado, Boulder
Yale University

Task Objective:

The objective of this research is to develop a fundamental understanding of aggregation and coalescence processes during electrically-driven migration of particles (or cells) and droplets.

Task Description:

The research includes the following tasks:

- Development of a theoretical description of electrically-driven particle aggregation by computing the relative velocity between two particles in near contact with hydrodynamic, electrokinetic, van der Waals, and electrostatic double-layer interactions, and by predicting the stability conditions and the rate of pair-wise aggregation in a semi-dilute suspension;
- Formulation of a description of electrically-driven drop coalescence by developing a simplified electrokinetic description of a charged fluid interface under thin double-layer conditions, and performance of initial computations for the interactions between a pair of electrically-driven droplets; and
- Observations of electrically-driven aggregation and coalescence by conducting terrestrial experiments to test the theoretical description of electrically-driven particle aggregation and observe electrically-driven droplet coalescence, with the results leading to future design of a flight-based experiment to gather quantitative observations for testing a theoretical description of electrically-driven aggregation and coalescence.

Task Significance:

The fundamental study of particle aggregation in electric fields is expected to have practical application to electrically-controlled cell flocculation for cell separation and recycle in space-based bioreactors, where gravity cannot be employed as has been previously done. Similarly, research conducted on drop interactions and coalescence is expected to provide an understanding of electrically-driven demixing of two liquid phases, such as those encountered in biphasic aqueous extraction of biological cells and molecules under reduced gravity when buoyancy-driven demixing is weak. Finally, the theoretical descriptions of two charged, migrating particles or drops are expected to have general scientific and engineering value.

Progress During FY 1996:

Trajectory analyses to compute stability diagrams and pairwise aggregation rates of small particles undergoing electrophoresis, sedimentation, or combined electrophoresis and sedimentation were completed. Particles aggregate more easily due to electrophoresis than due to sedimentation, but electrophoresis oriented in the opposite direction to sedimentation may completely stabilize a suspension of charged particles.

A model was developed for the migration of a surfactant-covered drop that remains spherical but the surfactant distribution is distorted by the applied field. This work was extended to the motion of a spherical particle with an arbitrary charge distribution embedded in an arbitrary electric field.

Zone electrophoresis experiments, in which a band of higher mobility particles passes through a band of lower mobility particles, were initiated. Aggregation occurs when the two bands coincide, creating a third band with doublets of intermediate mobility.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	0
MS Students:	1	MS Degrees:	1
PhD Students:	1	PhD Degrees:	0

TASK INITIATION: 2/93 **EXPIRATION:** 2/96**PROJECT IDENTIFICATION:** 962-24-08-10**NASA CONTRACT No.:** NAG8-945**RESPONSIBLE CENTER:** MSFC

Phase Segregation Due to Simultaneous Migration and Coalescence

PRINCIPAL INVESTIGATOR: Prof. Robert H. Davis

University of Colorado, Boulder

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to understand the interaction and coalescence of bubbles and drops due to thermocapillary and gravitational effects. Modeling is performed via population dynamics balances to predict the rate of phase segregation under the collective or individual action of the driving forces.

Task Description:

Significant effort is being devoted to the development and performance of ground-based experiments. The trajectories of interacting drops and the rate of phase segregation are being measured in a transparent immiscible liquid system under isothermal conditions.

Theoretical work is also being performed to predict the macroscopic phase separation and drop-size distributions due to buoyancy and thermocapillary motion and coalescence of immiscible dispersion of drops by solving the general population dynamics equations retaining both spatial and time dependencies.

Task Significance:

This research on phase segregation attempts to provide a predictive tool to determine the size distributions of drops in a heterogeneous immiscible fluid mixture. Inputs from other fundamental studies on drop interactions and coalescence are used in population dynamics models to predict the size distributions. This research will ultimately be of use in materials processing, food and beverage processing, and perhaps in the biotechnology industry.

Progress During FY 1996:

The focus of recent theoretical work has been on the effects of drop deformation on the interaction and coalescence of two drops in buoyancy driven motion. An asymptotic theory for small deformations has been completed and predicts that small deformations inhibit coalescence. Thus an attractive van der Waals force is necessary for coalescence. A fully three dimensional boundary integral numerical method has been developed for large deformations. Drops with moderate or large viscosity are predicted to elongate and break during the interaction while bubbles tend to align and eventually coalesce. Related work has also been completed on the interaction of two deformable drops in axisymmetric thermocapillary motion.

Experiments on the simultaneous coalescence and phase separation of a dispersion of drops undergoing gravitational motion have been completed and successfully compared to theory. It is observed that the rate of phase separation initially increases due to coalescence and later decreases when the large drops sediment out of the suspension.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 12/92 EXPIRATION: 11/95

PROJECT IDENTIFICATION: 962-24-05-39

NASA CONTRACT NO.: NAG3-138

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Wang, H. and Davis, R.H., Simultaneous sedimentation and coalescence of a dilute dispersion of small drops. *J. Fluid Mech.* 295, pp. 247-261 (October 1995).

Wang, H. and Davis, R.H., Collective effects of gravitational and Brownian coalescence on droplet growth. *J. Colloid Interf. Sci.* 178, pp. 47-52 (1996).

Wang, H. and Davis, R.H., Experiments on phase separation of dilute dispersions of coalescing drops. *J. Colloid Interf. Sci.*, 181, pp. 93-98 (1996).

Zhou, H. and Davis, R.H., Axisymmetric thermocapillary migration of two deformable viscous drops. *J. Colloid Interf. Sci.*, 181, pp. 60-72 (1996).

Zinchenko, A.Z., and Davis, R.H., Collision efficiency of drops and solid spheres in a shear flow at arbitrary Peclet numbers. *Phys. Fluids*, 7, pp. 2310-2327 (October 1995).

Presentations

Zinchenko, A.Z., Rother, M.A., and Davis, R.H., "Coalescence rate of slightly deformable drops in a gravitational field." AIChE Meeting, Miami, FL, November 1996.

Cell and Particle Interactions and Aggregation during Electrophoretic Motion

PRINCIPAL INVESTIGATOR: Prof. Robert H. Davis

University of Colorado, Boulder

CO-INVESTIGATORS:

Todd, P.

Task Objective:

The objectives of the proposed research are to develop an improved experimental method of quantifying electrophoretic aggregation, to extend the theoretical description to appropriately analyze and compare with the experimental results, to predict and test the combined effects of electrophoretic and Brownian aggregation of small particles, and to perform a preliminary design of a future flight experiment involving electrophoretic aggregation. This will be accomplished by performing the tasks in the following section.

Task Description:

Task 1 - Ground-based experiments on electrophoretic aggregation

In addition to improving our capabilities to observe individual doublet/aggregate formation in a uniformly mixed suspension, zone electrophoresis will be performed in which a band of higher-mobility particles will pass through a band of lower-mobility particles so that a third band, composed of heteroaggregates with intermediate mobility, is formed and quantified by light scattering or optical scanning. Gravity sedimentation and buoyancy effects will be partially suppressed in a portion of the experiments using a density gradient in a vertical configuration. The chambers will also be designed so that samples may be withdrawn and analyzed microscopically.

Task 2 - Microphysical theory of electrophoretic aggregation

Previous work on pairwise aggregation of particles with different zeta potentials in an electric field will be extended to combined gravity and electrophoretic motion (important for large particles), combined Brownian and electrophoretic motion (important for small particles), and to additional parameter values which include those of the suspensions used in the experiments. The combined gravity and electrophoretic motion is of particular interest, both because gravity sedimentation is expected to play a contributing role in the ground-based experiments and because it may be possible to suppress aggregation by appropriate manipulation of the relative orientation and magnitude of the gravity vector and the electric field.

Task 3 - Macrophysical theory of electrophoretic aggregation

In order to properly interpret the experimental results from zone electrophoresis and compare measured and predicted aggregation rates, a macroscopic theory capable of predicting the number density of aggregates versus position and time as one band passes through the other is needed. This will be accomplished using an inhomogeneous population dynamics model together with the collision kernels for pairwise aggregation predicted by the microphysical theory of Task 2. An interesting extension will be the analysis of the formation of multiplets comprised of many primary particles of two (or more) different zeta potentials. Unlike in gravity sedimentation, for which the aggregate velocity increases monotonically with aggregate size, the electrophoretic aggregate velocity is expected to be nearly size-independent and so relative motion and further aggregation may be suppressed once aggregates grow beyond some small size.

Task Significance:

Electrophoresis is widely used on the analytical scale (and sometimes on the preparative scale) for the separation of biological molecules such as proteins and nucleic acids. In order to improve the separation and reduce convection due to electrical heating, such separations are usually done in a gel matrix or a capillary tube. A suspension of particles or cells would clog a gel matrix or very fine capillary, however, and so free electrophoresis of the suspension is performed. In this case, the separation efficiency may be affected by three factors: (a) free convection or mixing due to thermal gradients, (b) particle sedimentation, and (c) particle aggregation. The proposed research will focus on particle aggregation due to electrophoretic motion with and without gravity sedimentation. The ground-based experiments will be designed to minimize free convection, but it is anticipated that a low-gravity environment will be needed to study electrophoretic aggregation in the absence of sedimentation and convection.

In addition to having general scientific and engineering significance, our fundamental study of particle aggregation in electric fields is expected to have practical application of electrically-controlled cell flocculation for cell separation and recycle in space-based bioreactors, where gravity cannot be employed. Similarly, an extension of the proposed study of drop interactions and coalescence would provide an understanding of electrically-driven demixing of two liquid phases, such as those encountered in biphasic aqueous extraction of biological cells and molecules under reduced gravity when buoyancy-driven demixing is weak.

Progress During FY 1996:

This is a new grant which was awarded May 1996. Graduate students have been hired and equipment has been ordered. Hardware set-up is currently in progress.

STUDENTS FUNDED UNDER RESEARCH:**TASK INITIATION:** 5/96 **EXPIRATION:** 5/00**PROJECT IDENTIFICATION:** 962-24-00**NASA CONTRACT No.:** NAG3-185**RESPONSIBLE CENTER:** LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Loewenberg, M. and Davis, R.H., Near-contact electrophoretic particle motion. J. Fluid Mech., 288, 103-122 (1995).

Theory of Solidification

PRINCIPAL INVESTIGATOR: Prof. Stephen H. Davis

Northwestern University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This work concerns our effort to understand - on a quantitative level - how various factors affect the morphology of solidification fronts and, hence, the resulting microstructures of the solidified material.

Task Description:

In the approach, nonlinear stability theory, asymptotic, and numerical methods are used to investigate the stability of the coupled systems describing the directional solidification of binary systems from the melt.

Task Significance:

The project aims at the theoretical prediction of microstructure in crystalline materials that would allow the a priori "design" of new materials. We will endeavor to answer the following central scientific question: How and under what conditions can crystals be grown in microgravity (mg) with different and "better" properties than those grown on Earth?

Progress During FY 1996:

Progress has been made in many areas of solidification. Three areas are of particular interest.

Schulze and Davis previously showed that on the basis of linear stability theory that substantial delay of morphological instabilities can be expected if during directional solidification the crystal is given certain prescribed motions. This shear stabilization has now been shown to extend into the nonlinear range. Thus, in the absence of gravity, "perfect" crystals should be able to be grown at substantially higher speeds. It is still an open question whether this stabilization exists, as on Earth, when buoyancy-driven convection is present.

If a convective flow is imposed upon a solidifying interface, then the morphology will be substantially affected. Presently, a two-dimensional steady case is being examined in order to determine how the intensity and wave length of the convection affect the onset of cellular growth.

If one wishes to study how a melt flow reacts to, say, the cellular corrugations of a solidifying interface, one requires a knowledge of the "effective" boundary conditions on long scales where the morphology has been "averaged away". Likewise, if one wishes to examine eutectic-growth instabilities and one could "average away" the eutectic scale, one could find a simple model for long-wave instabilities and the effect of fluid flow on these. Both of these efforts are in progress.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 10/87 EXPIRATION: 2/96

PROJECT IDENTIFICATION: 962-25-05-16

NASA CONTRACT NO.: NAG3-173

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Anderson, D.M., Worster, M.G., and Davis, S.H., The case for a dynamic contact angle in containerless solidification. *J. Crystal Growth*, (1996).

Hoyle, R., McFadden, G.B., and Davis, S.H., Pattern selection with anisotropy during directional solidification. *Phil. Trans. Roy. Soc.*, (1996).

Huntley, D.A. and Davis, S.H., Oscillatory and cellular mode coupling in rapid directional solidification. Phys. Rev. B , (1996).

Schulze, P. and Davis, S.H., Shear stabilization of a solidifying front: Weakly nonlinear analysis in the long-wave limit . (1996).

Schulze, T.P., and Davis, S.H., Effects of flow on morphological stability during directional solidification. Mat. Mater. Trans., (1996).

Skelton, A.C., McFadden, G.B., Impey, M.D., Riley, D.S., Cliffe, K.A., Wheeler, A.A., and Davis, S.H., On long-wave morphological instabilities in directional solidification. Euro. J. Appl. Math., (1996).

Presentations

Schulze, T.P., and Davis, S.H., "Long-wave weakly nonlinear theory for a directionally solidifying binary alloy in the presence of a time-periodic shear flow." Annual Meeting of the Division of Fluid Dynamics, American Physical Society, Irvine, October, 1995.

Theory of Solidification

PRINCIPAL INVESTIGATOR: Prof. Stephen H. Davis

Northwestern University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This work concerns our effort to understand - on a quantitative level - how various factors affect the morphology of solidification fronts and hence, the resulting microstructures of the solidified material.

Task Description:

In the approach, nonlinear stability theory, asymptotic, and numerical methods are used to investigate the stability of the coupled systems describing the directional solidification of binary systems from the melt.

Task Significance:

The project aims at the theoretical prediction of microstructure in crystalline materials that would allow the a priori "design" of new materials. We will endeavor to answer the following central scientific question: How and under what conditions can crystals be grown in microgravity (ug) with different and "better" properties than those grown on Earth?

Progress During FY 1996:

Progress has been made in many areas including the dynamics of triple junctions and the presence of departures from equilibrium, the shear stabilization of morphological fronts, the influences of surface-energy an isotropy on patterns in directional solidification, and the dynamics of eutectic growth.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NAG3-173

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Anderson, D.M. and Davis, S.H., The spreading of volatile liquid drops on heated surfaces. *Physics of Fluids*, vol. 7, pp. 248 (1996).

Anderson, D.M., Worster, M.G., and Davis, S.H., The case for a dynamic contact angle in containerless solidification. *Journal of Crystal Growth*, vol. 163, pp. 329 (1996).

Hoyle, R. McFadden, G.B. and Davis, S.H. Pattern selection with anisotropy during directional solidification. *Transaction of the Royal Society London*, (in press).

Schulze, T.P. and Davis, S.H. The influence of oscillatory and steady shears on interfacial stability during directional solidification. *Journal of Crystal Growth*, vol. 143, pp 317 (1995).

Schulze, T.P. and Davis, S.H., Shear stabilization of morphological instability during directional solidification. *Journal of Crystal Growth*, vol. 149, pp. 149 (1995).

Schulze, T.P. and Davis, S.H. Shear stabilization of a solidifying front: Weakly nonlinear analysis in the long wave limit. *Physics of Fluids*, (in press).

Schulze, T.P. and Davis, S.H. Effects of flow on morphological stability during directional solidification. *Metallurgical and Materials Transactions*, (in press).

Microgravity Foam Structure and Rheology

PRINCIPAL INVESTIGATOR: Prof. Douglas J. Durian

University of California, Los Angeles

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to investigate the origin of the most striking and least understood rheological properties of foam by measuring elastic and flow behavior for a sequence of aqueous foams with increasing liquid content. The microscopic structure and dynamics of the foams will simultaneously be characterized by recently developed multiple light scattering techniques.

Task Description:

Foam structure and dynamics will be measured directly and non-invasively through development and use of novel light scattering techniques such as Diffusing Wave Spectroscopy (DWS). Foam rheology will be measured in a custom rheometer which allows simultaneous optical access for multiple light scattering. Microgravity conditions will ultimately be required to eliminate the increasingly rapid gravitational drainage of liquid from in between gas bubbles as the liquid:gas volume fraction is increased toward the rigidity-loss transition.

Task Significance:

This experiment will constitute the first measurement of how the surprising solid-like elastic quality of foam vanishes as the volume fraction of liquid is increased. The simultaneous measurements will also permit the first quantitative correlation of macroscopic rheological behavior with the underlying microscopic structure and dynamics, thus providing new insight into the origin of the dual solid/liquid nature of foams.

Progress During FY 1996:

During this period we have achieved important goals in both using and developing the multiple light scattering diagnostics. As for the techniques themselves, we have incorporated the effects of refraction and angle-dependent wall reflectivity into our previous diffusion theory prediction for the angular dependence of diffusely transmitted light. And we have verified the result both by random walk computer simulations and by experiments on known suspensions of colloidal spheres and on aqueous foams. We have also developed two new approaches to the theory of diffusing light spectroscopies in order to significantly improve the accuracy with which data may be analyzed for thin samples, for short times, and for cases of strong absorption and anisotropic scattering. As for the physics of foams, we have fully characterized an earlier puzzling observation of short-time nonexponential dynamics in the diffusing-wave spectroscopy signal. By altering the rate of bubble rearrangements, both by application of shear and by change of ambient temperature, we have identified the origin of the short-time dynamics as thermal fluctuations of the liquid-gas interfaces. By two independent analyses we extract a single consistent amplitude for this thermal motion, and can relate it to the macroscopic shear modulus of the foam. These experiments and the new theories will all be important in analyzing the multiple light scattering diagnostic data obtained in flight. On a separate front we also have conducted further simulations of the model of foam rheology I recently introduced based on the approximation of pairwise bubble-bubble interactions. This work gives theoretical insight into the precise nature of how the unusual elastic character of foams melts away with increasing liquid content. It will provide an important benchmark for comparison with the ultimate flight experiments.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 3

TASK INITIATION: 1/93 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-24-05-73

NASA CONTRACT NO.: NAG3-141

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Durian, D.J., Two-stream theory of diffusing-light spectroscopies. *Physica A* , 229, 218-235 (1996).

Durian, D.J. and Rudnick, J., Photon migration at short times and distances and in cases of strong absorption. *J. Opt. Soc. Am A*, (1996).

Gopal, A.D. and Durian, D.J., Fast thermal dynamics in aqueous foams. *J. Opt. Soc. Am A*, (1996).

Vera, M.U. and Durian, D.J., The angular distribution of diffusely transmitted light. *Phys. Rev. E* 53, 3215-3224 (1996).

Presentations

Durian, D., "Foam structure and rheology." University of Illinois at Champagne-Urbana, Dept. of Theor. & App. Mech., 1996.

Durian, D., "Foam structure and rheology." University of Michigan, Dept. of Physics, 1996.

Durian, D., "Foam structure and rheology." University of Pennsylvania, Dept. of Physics, 1996.

Durian, D., "Foam structure and rheology." University of Pittsburgh, Dept. of Physics, 1996.

Durian, D., "Foam structure and rheology." College de France, 1996.

Durian, D., "Foam structure and rheology." Universit=E9 de Strasbourg, LUDFC and Institut de Physique, 1996.

Durian, D., "Foam structure and rheology." Institut Curie, 1996.

Magnetothermal Convection in Nonconducting Diamagnetic and Paramagnetic Fluids

PRINCIPAL INVESTIGATOR: Prof. Boyd F. Edwards

West Virginia University

CO-INVESTIGATORS:

Gray, D.O.

West Virginia University

Task Objective:

The objectives of this project are to obtain a full theoretical understanding of the continuum forces exerted by magnetic fields on fluids which do not conduct electricity and to evaluate the potential of these forces to control and position fluids in microgravity environments.

Task Description:

The equations governing the motion of non-conducting, non-magnetic fluids in magnetic fields will be rigorously justified. Analytical solutions will be obtained for horizontal and vertical layers of fluid subjected to non-uniform temperatures and magnetic fields, and they will be compared with previous experimental data. Similarity solutions for thermal plumes in non-uniform magnetic fields will be completed. The "magnetic curtain" effect reported by Japanese investigators will be explained. A commercial computational fluid dynamics computer code will be modified to incorporate magnetic forces so that flow in realistic geometries can be studied. A ground-based experiment will be designed in which magnetic forces will be used to simulate a microgravity environment. Potential applications of magnetic forces on spacecraft will be explored.

Task Significance:

Magnetic forces offer the potential to create arbitrary, controllable body forces in paramagnetic fluids such as gaseous and liquid oxygen. Similar, though weaker forces can be created in diamagnetic fluids such as nitrogen and water. These forces may need to be allowed for when precise measurements of fluid properties are made. Magnetic forces could be used to mimic gravity, to pump and position fluids, or to counteract g-jitter.

Progress During FY 1996:

This report covers the first three weeks since funding was received. Note that Dr. Boyd Edwards and Dr. Donald Gray are equal co-principal investigators.

Postdoctoral Fellow Dr. Jie Huang has performed a linear stability analysis of a horizontal layer of paramagnetic fluid heated from below in a uniform magnetic field. The applied field was found to have a combined null effect on the buoyancy-driven convective instability when the field is 45° above or below the horizontal. The field suppresses convection when it is within 45° of the horizontal, and enhances convection otherwise.

The final selection of the personal computer hardware and computational fluid dynamics software is nearly complete.

The rigorous justification of the expression for the magnetic body force and an improved solution for magnetothermal convection between vertical surfaces are in progress.

The conceptual design of a ground-based experiment is well underway. The investigators visited the renowned experimentalist Dr. Paul Kolodner of Lucent Technologies (formerly Bell Labs) to discuss details of the experimental design.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/96 **EXPIRATION:** 6/98**PROJECT IDENTIFICATION:** 962-24-00**NASA CONTRACT NO.:** NAG3-192**RESPONSIBLE CENTER:** LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Edwards, B.F., Gray, D.D., and Huang, J., "Magnetothermal convection in nonconducting diamagnetic and paramagnetic fluids." paper presented at the Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 13-15, 1996.

Huang, J., Edwards, B.F., and Gray, D.D., "Thermoconvective instability of paramagnetic fluids in a uniform magnetic field." abstract presented to the Annual Meeting of the Division of Fluid Dynamics, American Physical Society, 1996.

Effects of Gravity on Sheared Turbulence Laden with Bubbles or Droplets

PRINCIPAL INVESTIGATOR: Prof. Said E. Elghobashi

University of California, Irvine

CO-INVESTIGATORS:

Lasheras, J.

University of California, San Diego

Task Objective:

The main objective of this numerical/ experimental study is to improve the understanding of the physics of two-way coupling between the dispersed phase and turbulence in a homogeneous turbulent shear flow laden with small liquid droplets (in gas) or gaseous bubbles (in liquid).

Task Description:**Numerical**

The method of direct numerical simulation (DNS) is used to solve the full three-dimensional, time-dependent Navier-Stokes equations including the terms describing the two-way coupling between the dispersed phase and the carrier flow. The results include the temporal evolution of the three-dimensional energy and dissipation spectra and the rate of energy transfer across the energy spectrum to understand the fundamental physics of turbulence modulation, especially the effects of varying the magnitude of gravitational acceleration. The mean-square displacement and diffusivity of the droplets (or bubbles) of a given size and the preferential accumulation of droplets in low vorticity regions and bubbles in high vorticity regions will be examined in detail for different magnitudes of gravitational acceleration. These numerical results which will be compared with their corresponding measured data will provide a data base from which a subgrid-scale (SGS) model can be developed and validated for use in large-eddy simulation (LES) of particle-laden shear flows.

Experimental

Two parallel sets of experiments will be conducted: bubbles in an immiscible liquid and droplets in air. In both experiments homogeneous shear will be imposed on the turbulent carrier flow. The instantaneous velocities of the fluid and polydispersed-size particles (droplets or bubbles) will be measured simultaneously using a two-component Phase-Doppler Particle Analyzer (PDPA). Also, the velocity statistics and energy spectra for the carrier flow will be measured.

Task Significance:

Turbulent, dispersed, two-phase flows occur in a wide range of manufacturing and processing applications. Often, the efficiency of the process depends directly on the degree of uniformity of dispersion of one phase into the other, e.g. the dispersion of liquid droplets in a gas, or gaseous bubbles in a liquid. Our recent numerical simulations indicate that gravity reduces dispersion of particles in turbulent shear flows. Thus, when the influence of gravity is reduced or eliminated, it is expected that the efficiency of many of these manufacturing or chemical processes could be greatly enhanced. However, at present, no existing two-phase mathematical model (i.e. not direct numerical simulation) is accurate enough to be used for the design, operation and control of processes involving turbulent, dispersed two-phase flows. The aim of this project is to provide the necessary data to develop reliable mathematical models.

Progress During FY 1996:**Numerical**

During the past three months (i.e. since the the start of this project) we have completed the simulation of the dispersion of particles in homogeneous shear flow in the one-way coupling regime (i.e. the particles do not affect the turbulence). These particles are spherical and of uniform size. We also started the two-way coupling simulation of particles in a homogeneous shear flow.

Experimental

Experiment 1 . Measurements of particles/turbulence interaction in homogeneous isotropic turbulent flows : Part I. droplets in air; Part II. bubbles in water.

Experiment 2 . Measurements of particles/turbulence interaction in homogeneous turbulent shear flows:

- Part I. droplets in air;
- Part II. bubbles in water.

During the past three months we have completed the construction of the two main experimental facilities needed for Experiment 1, Parts I and II. The facility for Part I consists of a uniform flow, blow-down wind tunnel to study the modification of decaying homogeneous turbulence by droplets of a known size distribution and volume fraction. The second facility, to be used in Part II, is a water channel conceptually identical to the above wind tunnel except that the dispersed phase consists of bubbles and the carrier fluid is water.

Using a combination of a Laser Doppler Velocimeter (LDV) and a Phase Doppler Particle Analyzer (PDPA), we have already completed the first set of detailed measurements of the effect of the dispersed phase on the evolution of the carrier flow turbulence. The experimental data are being analyzed at present. Direct Numerical Simulation (DNS) of this flow is conducted in parallel so that the combined numerical/experimental study will provide detailed information about the particle/turbulence two-way coupling interaction in homogeneous isotropic turbulent flows.

The experiment of Part II is currently underway. It is expected that this part will take about 5 months due to the experimental difficulties arising from the presence of bubbles. Also simultaneous DNS studies are performed for flow conditions identical to those of the experiment.

In addition to the above described progress in the 1g experimentation, we have begun the preliminary design of a microgravity facility to investigate bubble/turbulence interaction and the dynamics of bubbly flows in environments representative of two-phase flows encountered in microgravity applications.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NAG3-183

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Ahmed, A.M. and Elghobashi, S.E., Direct numerical simulation of particle dispersion in homogeneous turbulent shear flows. *Journal of Fluid Mechanics*, (July 1996).

Elghobashi, S.E. and Lasheras, J., Explosive breakup of a liquid jet by a swirling coaxial gas jet. *Physics of Fluids*, vol. 8, no. 7, p 1696 (July, 1996).

Evaporation, Boiling, and Condensation on/in Capillary Structures of High Heat Flux Two-Phase Devices

PRINCIPAL INVESTIGATOR: Prof. Amir Faghri

University of Connecticut

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective is to investigate the fundamental phenomena that dictate the design of various two-phase heat transfer devices for high-heat flux and zero-g applications.

Task Description:

Theoretical analyses will be carried out on 1) the formation of vapor phase and vapor-liquid interfaces in a porous structure, 2) formation of thick expended liquid films during evaporation, 3) liquid and vapor flow in/over an evaporating meniscus, and 4) the role of vapor-liquid interaction and capillary forces during condensation.

Experiments on miniature heat pipes (0.1 x 0.2 mm grooves in 2.5x10x120 mm heat pipes), with and without porous metal coatings, would be carried out to visualize fluid flows and study the evaporation, boiling and condensation processes.

Studies on glass capillary tubes with semi-transparent heaters, and cylindrical micro heat pipes would be carried out; from the results of these, and other ground-based experiments, operational conditions for future zero-g experiments would be developed.

Task Significance:

Thermal control elements such as heat pipes, capillary pumped loops, loop heat pipes, evaporators, and condensers employ "capillary porous structures" especially in the design of high heat-flux and zero-g applications. This experimental and theoretical investigation centers on fundamental study of this "capillary porous structures".

Progress During FY 1996:

This is a new grant starting in FY96.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 2
MS Students: 2
PhD Students: 1

TASK INITIATION: 5/96 **EXPIRATION:** 5/00**PROJECT IDENTIFICATION:** 962-24-00**NASA CONTRACT NO.:** NAG3-187**RESPONSIBLE CENTER:** LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Faghri, A. and Khrustalev, D., "Evaporation, boiling and condensation on/in capillary structure of high heat flux two-phase devices." Proceedings of the Third Microgravity Fluid Physics Conference, Cleveland OH, June 13-15, 1996.

The Influence of Gravity on Nucleation, Growth, Stability and Structure in Ordering Soft-Spheres

PRINCIPAL INVESTIGATOR: Prof. Alice P. Gast

Stanford University

CO-INVESTIGATORS:

Pine, D.J.

Exxon Research & Engineering

Task Objective:

Our goal is to understand the dynamics of particles within colloidal crystals. In particular, we focus on the influence of the cell walls and gravity on the particle dynamics. In this study, we will use a novel light scattering experiment, known as diffusing wave spectroscopy, to probe particle motions in turbid suspensions. This is a noninvasive experimental probe of interparticle dynamics.

Task Description:

Aqueous suspensions of charged colloidal particles provide attractive model systems for the study of crystal dynamics due to the long range Coulombic repulsion that diminishes the influence of hydrodynamic interactions in the suspension. In this system of charged polystyrene latex synthesized in our laboratory with ionic comonomers, we can observe and provoke homogeneous nucleation to two crystal lattices. We can also study twinning and a crystallization growth instability analogous to those observed in molecular systems. These phenomena motivate and provide a means for us to investigate the role of interfacial tension, surface interactions and gravity on the crystallization process. A key feature of this study is the use of density matching experiments to study crystal growth without the influence of gravity. We suspend our particles in mixtures of deuterated and normal water to render them neutrally buoyant. We focus our investigation on the dynamics of particles in colloidal crystals using light scattering as our measurement tool. Future studies on more dense colloidal particles would require low gravity experiments.

Task Significance:

An important fundamental feature of this work is the application of diffusing wave spectroscopy to ordered suspensions. This has potential implications for the study of other interesting systems such as liquid crystals or protein arrays. Our combination of experimental and theoretical treatments provides a means to interpret the dynamics of particles in a lattice through the analysis of the multiply scattered light interacting with the array. This study will provide a test of our understanding of crystalline dynamics, the influence of external fields such as produced by walls or gravity and the nature of crystal defect formation.

Progress During FY 1996:

In this program we aim to investigate the influence of gravity on particle dynamics in colloidal crystals. Our system is an electrostatically stabilized suspension of polystyrene lattices in water. We control the interparticle interactions and hence the suspension structure and dynamics through the ionic strength of the suspending aqueous fluid. Unfortunately, such suspensions are quite opaque and require the multiple scattering technique known as diffusing wave spectroscopy (DWS) for their interrogation. We have extended this approach by developing a spatially resolved (SR-DWS) method capable of handling ordered colloidal suspensions. This novel scattering geometry with its variable incident beam and detector positions allows us to characterize the propagation of the diffusing light over different length scales.

We developed a mathematical analysis of the problem of light diffusing from a point source into a semi-infinite solid. The resulting autocorrelation function depends on the distance of our point detector from the point source and thus allows us to perform a series of experiments to test the diffusion model for ordered arrays. We illuminate the front face of our suspension with a focused beam of an Argon ion laser. The detection occurs through a 0.2 mm fiber optic cable located at a variable distance from the point source. The source to detection distance ranges from 400 to 3500 micrometers; ordered samples require the longer distance measurements to ensure that the light is fully diffusing. The autocorrelation function is calculated on a high-speed correlator.

We have shown that the autocorrelation function obtained from the diffusing photon model gives excellent agreement with the measured autocorrelation functions. This confirms the diffusive photon transport in both disordered and ordered samples; however, the transport mean free path is much larger for the ordered samples than

for the disordered ones. This suggests that the optical transport in these suspensions is primarily affected by structures on length scales smaller than the size of the individual crystallites but much larger than the crystal lattice spacing.

Our fitting procedure also yields a measurement of the characteristic dynamic processes in the suspension through the relaxation time. We observe a dramatic enhancement in the dynamics for ordered suspensions. In contrast to the results for the transport mean free path, we see a dependence of the ordered dynamics on the suspension ionic strength. This suggests that the dynamic processes are primarily governed by structures and interactions on the length scale of the lattice.

We have also observed for the first time underdamped lattice modes at long times in the autocorrelation functions. These modes could not be observed in other experiments due to the thin sample cells used. Our new DWS geometry allowed us to measure these modes without the influence of confining walls. The analysis of these modes serves as a test of the harmonic lattice model.

Our new SR-DWS scattering experiment has given us a tool for properly interrogating ordered colloidal suspensions. The spatial resolution that it provides allows us to more fully characterize the suspension to obtain accurate measurements of its optical and dynamic properties. We have shown its applicability to ordered colloidal suspensions, but it should be equally useful for interrogating any number of other anisotropic systems such as those composed of anisotropic particles. This new modification to the DWS formalism will hopefully make it more applicable to a wider variety of experimental systems with the Laser Light Scattering facility being developed at NASA Lewis Research Center.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 0

PhD Students: 1.3

TASK INITIATION: 7/94 EXPIRATION: 7/96

PROJECT IDENTIFICATION: 962-24-05-83

NASA CONTRACT NO.: NAG3-165

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Gast, A.P., "Dynamics of ordered and disordered colloidal suspensions." paper presented by A. Gast, American Institute of Chemical Engineers, Miami Beach, Florida, November 1995.

Nilsen, S.J., "Structure and dynamics in ordered and disordered colloidal suspensions." Dissertation, Stanford University, March 1996.

The Influence of Gravity on Colloidal Crystallization and Field-Induced Aggregation

PRINCIPAL INVESTIGATOR: Prof. Alice P. Gast

Stanford University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The goal of this research is to understand the influence of gravity on concentrated suspension processes including colloidal crystallization and field induced aggregation. Applying light scattering techniques to these problems we seek to investigate the fundamental particle motions in such systems in an effort to relate dynamics to changes in structure and interactions.

Task Description:

Magnetorheological (MR) fluids are suspensions of colloidal particles which acquire dipole moments when subjected to strong magnetic fields. We study particle dynamics in an MR fluid using diffusing-wave spectroscopy (DWS), a light scattering technique which was developed to probe opaque suspensions. With DWS we measure the fluctuations of multiply scattered light caused by phase changes from the motion of the scattering particles. An autocorrelation of the fluctuation is computed using a high speed correlator. The decay time of the autocorrelation function gives information about the particle dynamics. Because light is scattered many times as it diffuses through the sample, DWS is sensitive to very small displacements of the scattering particles. We combine these investigations with simulations of particle motions in external fields.

Task Significance:

Magnetorheological (MR) fluids are suspensions of colloidal particles which acquire dipole moments when subjected to strong magnetic fields. In dilute suspensions the dipolar particles aggregate to form long chains. More concentrated systems exhibit a rapid liquid to solid transition as chains cross-link, and are capable of supporting stresses perpendicular to the applied field. These unique properties have many possible technological applications, especially for actuator-type devices. While several studies have aimed to describe the rheological properties of MR fluids on a microstructural basis, we seek to investigate the fundamental particle motions of such systems in an effort to relate dynamics to changes in structure and interactions. Additionally, the ability to experimentally probe colloidal suspensions interacting through tunable anisotropic potentials is of fundamental interest.

Progress During FY 1996:

During this fiscal year, we have developed an apparatus to study the dynamics of MR fluid suspensions. We have also made the first nearly neutrally buoyant suspensions of paramagnetic emulsion particles. We measured the decay of the autocorrelation function first for freely-diffusing MR particles then we applied a static magnetic field, and measured the autocorrelation function at various time intervals as the particles aggregate to form dilute chains. Various particle interaction strengths were tested by changing the static field strength. The absorption of light by the particles was independently measured and incorporated into the analysis. We have also taken into account changes in the optical properties of the system during aggregation.

The decay time of the autocorrelation increases when a static field is applied to the MR fluid. The increase is low in magnitude and independent of chain length for all interaction strengths; however, it increases with field strength. These observations can be attributed to Brownian motion of a particle on a flexible chain of beads and springs. The increased decay time is due to the particle confinement on the chain, with the constraint enhanced by increasing interaction strengths. Using computer simulations, we calculated the mean-squared displacement of particles on a model bead-spring chain at two interaction strengths. The expected decay times from the simulations agree favorably with our experimental results.

In the near future, we will improve our density matching between particles and solvent in order to investigate cross-linked systems without sedimentation. Also, the sensitivity and accuracy of the scattering measurements will be improved by changing our MR suspension.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 0

PhD Students: 1

TASK INITIATION: 7/96 **EXPIRATION:** 7/00**PROJECT IDENTIFICATION:** 962-24-00**NASA CONTRACT NO.:** NAG3-188**RESPONSIBLE CENTER:** LeRC

Material Instabilities in Particulate Systems

PRINCIPAL INVESTIGATOR: Dr. Joe D. Goddard

University of California, San Diego

CO-INVESTIGATORS:

Didwania

University of California, San Diego

Task Objective:

To investigate the instability of spatially homogeneous deformation processes in fluid-particle and granular media systems. Specific emphasis will be on two particular areas: 1) dilatational and shearing instabilities in dense particulate suspensions; and 2) dissipative clustering in rapid granular shear flows.

Task Description:

The work anticipated will mainly be theoretical in nature, guided by computer simulation. Kinetic-theory analyses will be performed from which continuum models will be extracted. The work will be divided up into three tasks. Task 1 will involve the computer simulation of the quasi-static granular mechanics in dense particulate suspensions accounting for strain localization and other spatial inhomogeneities. Task 2 will entail theoretical modelling and experimental investigations relative to fluid-saturated granular media; and in particular the development of experimental photochromic particle visualization techniques. Task 3 will consist of the analysis of clustering instabilities in low-density rapid granular flows modelled by non-Newtonian constitutive equations.

Task Significance:

Particulate dispersions and granular media represent an interesting and important class of materials that occur in natural as well as technological settings. Such media are intriguing because they exhibit many similarities with molecular systems, including transitions from solid-like to fluid-like behavior; yet they involve strongly dissipative behavior at the particle level. The underlying physical phenomena are important for understanding the mechanics of particulate matter in a number of natural and technological fields, including sandy soils and granular rock masses in geomechanics; as well as various powders and metallurgical or ceramic precursors in materials processing.

Progress During FY 1996:

The progress to date will be delineated by Tasks as defined above.

Task 1. Based on a quasi-static computer simulation developed under a previous grant, computations are now being completed of the Reynolds dilatancy and plastic yield surfaces for various proportional loading histories. A substantial paper is in the final stages of preparation. Modifications to these computer simulations will be made later in the year to allow for the descriptions of material instabilities and shear bands.

Task 2. Again continuing the work of a previous grant, this effort continues the development of refractive index matched fluid particle systems with transparent particles made from photochromic glass doped with photochromic dye. At present, highly transparent index-matched dispersions of crushed photochromic glass in ZnCl solutions have been made; and an optical system to create a collimated UV beam for photochromic excitation of tracer particles is under construction.

Task 3. Efforts have begun in developing general theories of material stability for low-density rapid granular flows and in dense particulate suspensions in viscous fluids. For the latter, an interesting shear-banding instability has been theoretically predicted in work to date.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 0

TASK INITIATION: 1/96 **EXPIRATION:** 12/98**PROJECT IDENTIFICATION:** 962-24-00**NASA CONTRACT NO.:** NAG3-188**RESPONSIBLE CENTER:** LeRC

Thermoacoustic Effects at a Solid-Fluid Boundary: The Role of a Second-Order Thermal Expansion Coefficient

PRINCIPAL INVESTIGATOR: Dr. Ashok Gopinath

Naval Postgraduate School

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective is to analytically and numerically study the steady state transport of momentum and energy due to thermoacoustic streaming from an intense acoustic field incident on a rigid boundary in the absence of gravity. The effort will explore the role of the second order thermal expansion coefficient, viscous dissipation, and compressibility work.

Task Description:

The work is broken up into three years. The first year will focus on setting up the analytical form of the momentum and energy equations of motion appropriate in cylindrical coordinates. This will involve first and second order equations of motions to deal with the inner Stokes boundary layer. A suitable equation of state will be defined to enable first and second order description of density fluctuations in the host fluid. Leading order solutions will be derived for the respective equations of motion in the inner Stokes region.

The second year will consist of further analytical work. Streaming, density fluctuations, and the importance of the second order thermal expansion coefficient will be calculated. Proper handling of large streaming Reynolds numbers will be verified. The form of the matching boundary conditions for the inner and outer Stokes boundary layers will be determined.

The third year will be primarily numerical work. The equations of motion for the outer Stokes region will be finalized. The discretized equations will then be coded and run. Allowance for a finite heat capacity in a solid sphere being levitated will be included as time allows. Also a fluid hard sphere will also be considered as time allows to explore internal flows in a levitated body.

Task Significance:

This work is supportive of a more thorough understanding of heat transfer and generation in microgravity experiments using acoustic levitation as well as the broader application of thermoacoustic engines in refrigeration.

Progress During FY 1996:

No progress to report for FY96 since the PI requested and was awarded support to start at the beginning of FY97.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/96 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NAG3-185

RESPONSIBLE CENTER: LeRC

Fluid Mechanics of Capillary Elastic Instabilities in the Microgravity Environment

PRINCIPAL INVESTIGATOR: Prof. James B. Grotberg

Northwestern University

CO-INVESTIGATORS:

Halpern, D.

University of Alabama

Task Objective:

The research proposed in this application addresses the capillary-elastic instabilities of liquid-lined flexible tubes in the presence of variable surface tension due to heat or surfactants. Three important applications of this fundamental problem are 1) closure and reopening of small airways in the lung, 2) annular extrusion processes, and 3) two-phase flow in porous and poro-elastic materials.

Task Description:

The project will address coupled fluid-elastic instabilities of a flexible tube coated internally with a thin liquid film by both theoretical and experimental means. The theoretical analysis of closure leads to non-linear, coupled evolution equations which will be solved numerically. The simplest system will be treated first, followed by increasingly more complex modelling of fluid and wall properties, surfactants and geometry. We will analyze a mathematical model of post-closure filling flows and reopening phenomena using a similar approach as the closure problem. An experiment of a flexible tube containing a thin liquid layer on its wall and a liquid core of a much smaller viscosity but similar density is proposed. This will eliminate, as much as possible, effects of gravity on the instability which will be recorded on video tape and analyzed for growth rates, stability criterion, filling flow behavior and reopening. Effects of surfactant in this experiment will be analyzed.

Task Significance:

The fluid mechanical phenomena being addressed in this project pertain to the closure of small airways in the lung. Airway closure is of significance in gas exchange and has important dependencies on gravity. When airways close, often near the end of expiration, the transfer of gases into and out of the blood stream is no longer possible for the affected lung units. The airway can then reopen when inspiration occurs. Microgravity will likely make airway closure more prevalent, due to smaller lung sizes, and more uniform. This is potentially a significant change in lung physiology for astronauts under various conditions. Low pressure space suits, which have high oxygen concentrations, may exacerbate airway closure.

In addition to the pulmonary application, this research addresses issues which are basic to other engineering fields. As a technologically related example, there are two air-liquid free surfaces in annular extrusion methods for manufacturing small hollow fibers. These may be materials processed for a number of applications. Also, there are methods of coextrusion manufacturing (e.g., optical fibers) in which there is an inner plug core of liquid and an outer annulus of a different liquid extruded simultaneously, one around the other. Understanding the coupled behavior of our problem will shed light on these materials processing examples, since the approaches will have many commonalities and the stability behavior is likely to overlap in certain parameter ranges where one surface is more unstable than the other, for example.

Among the other important engineering applications of these investigations is the development of models of two-phase flow in porous media where surface tension phenomena modify the connectivity of the fluid phases and thereby affect the overall flow behavior. Oil recovery from porous rock is a typical application of such models and is a limiting case of our work for rigid walls. We will provide new modelling on the more general problem of interfacial flows in poroelastic media, and important engineering and technological field.

Progress During FY 1996:**Airway Closure - Capillary-Elastic Instabilities****Effects of Forced Oscillations**

Forced oscillations of the capillary instability which causes closure of a fluid cylinder (Rayleigh instability) is an important aspect of respiration and fiber extrusion. Respiratory movement causes a cycling of the air flow over the

liquid film coating the airways and stretching of the airway radius and length. The motivation is to understand how the breathing frequency (in high frequency ventilators, for example) can affect airway closure instabilities. In fiber extrusion, forced oscillations of the flow device have been investigated to reduce the likelihood of instabilities which adversely affect the manufactured fiber.

Two types of forced oscillatory perturbations have been studied in our work: 1. sinusoidal oscillations of the tube radius and, 2. oscillatory shear stress at the air-liquid interface. The oscillations become apparent in the evolution equations through two parameters, these being the dimensionless oscillatory frequency Ω , and the dimensionless amplitude of the oscillations d (which is a measure of the tidal volume). The three evolution equations were solved numerically using a Crank-Nicolson finite difference time marching scheme. The stability of the system was henceforth determined, thus giving closure times as a function of breathing frequency Ω , and tidal volume d . Results for the radial oscillations, show that the closure time is reduced when the system is oscillated with a finite frequency Ω . In the oscillatory frequency range where the system is independent of the initial conditions, the closure time is independent of the frequency of oscillations. It is, however, dependent on the tidal volume d ; the airway closure time decreasing as d is increased. These results indicate that the destabilizing effect of expiration (thicker liquid lining) is greater than the stabilizing effect of inhalation. Our results for the imposed oscillatory shear stress at the air-liquid interface are currently limited to linear theory for the growth rates of instabilities. Preliminary results indicate that the most dangerous wave number (fastest growing wave) is modified by the shear and, for some values of the imposed shear-oscillation amplitude and frequency, more than one wave number can have maximal growth rates. Hence a mode coupling appears to be possible.

Effect of wall permeability

An important airway wall property in the lung is that there is a liquid source from the underlying cells and tissue. We have extended our unperturbed airway closure model to include a wall source of fluid which flows due to simple transmural pressure differences and a permeability constant. Our preliminary results show that wall permeability can have a significant effect on airway closure. Depending on the magnitude of the surrounding tissue pressure and the permeability constant, several scenarios are possible. The capillarity instability can be enhanced, diminished, and sometimes it can even be prevented all together.

Airway Reopening - Liquid Plug Transport

When the lung's liquid lining is too thick, surface tension instabilities cause a liquid bridge or plug to form, a phenomena we have studied extensively in the context of airway closure. This plug will propagate along the airway by gravity drainage and by pressure drops imposed across it during respiration or mechanical ventilation. As it does, it leaves behind a thin liquid film whose thickness depends on how fast the bolus is moving. If the thickness of the trailing film exceeds that of the liquid lining ahead of the bolus, then the bolus must decrease in volume as it propagates, leading ultimately to reopening of the airway. If it does not, then the liquid bridge will continue to obstruct the airway. We have developed a model of the propagation of a liquid bolus along an elastic tube. Given the precursor layer thickness and the imposed pressure drop across the plug, the propagation speed of the bolus and the trailing film thickness can be found. We have found that increased wall flexibility decreases the critical pressure drop required for eventual rupture, i.e. makes the tube easier to open.

Progress in Experiments

Annular Film Closure in Capillary Tubes

Using video-microscopy, we have been examining the instabilities of an annular film of oil with a water core within a capillary tube. The dimensionless parameters in this system approximate well the air-liquid interface of the lung. The film thickness can be observed to develop over time until the capillary instability causes closure. When we include surfactants in the system, it prolongs the closure time and allows for thicker films to be more stable. The initial growth rates and time to closure are now being compared to our theoretical predictions and preliminary results indicate a good correlation. Eventually we will examine a flexible tube and one with forced oscillation.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	1
PhD Students:	1	PhD Degrees:	0

TASK INITIATION: 6/94 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 962-24-05-84

NASA CONTRACT NO.: NAG3-163

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Gaver, D.P., Halpern, D., Jensen, O.E., and Grotberg, J.B., Fluid-structure interactions of bubble motion through a compliant channel - a model of pulmonary airway reopening. *Euromech*, London, England, 344, (April 1996).

Gaver, D.P., Halpern, D.M., Jensen, O.E., and Grotberg, J.B., The steady motion of a semi-infinite bubble through a flexible-walled channel. *J. Fluid Mech.*, 319, 25-65 (1996).

Moriarty, J.A. and Grotberg, J.B., Flow induced instabilities of a mucus-serous bilayer. *Euromech*, London, England, 344, (April 1996).

Presentations

Gaver, D.P., Perun, M.L., Halpern, D., and Grotberg, J.B. "The influence of airway wall mechanical properties on airway reopening pressures and wall stresses." *Biomedical Engineering Society Annual Fall Meeting*, Boston, MA, October 1995.

Grotberg, J.B. and Howell, P.D., "The propagation of a liquid bridge through an elastic tube and airway reopening." *Biological Fluid Mechanics Symposium, ASME Mechanics and Materials Conference*, Baltimore, June 1996.

Halpern, D., Grotberg, J.B., and Jensen, O.E., "Surfactant spreading in a simple long model." *American Physical Society, Division of Fluid Dynamics, 49th Annual Meeting*, Irvine, CA, November 1995.

Howell, P., Cassidy, K., Gavriely, N., Glucksberg, M., and Grotberg, J.B., "Airway reopening: theoretical and experimental studies." *Experimental Biology '96*, Washington, D.C., April 1996.

Howell, P.D. and Grotberg, J.B., "The propagation of a liquid bridge through an elastic tube and airway reopening." *Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH*, June 13-15, 1996.

Mariarty, J.A. and Grotberg, J.B. "A model of flow-induced instabilities of mucus." *American Physical Society, Division of Fluids Dynamics, 48th Annual Meeting*, Irvine, CA, November 1995.

Moriarty, J.A. and Grotberg, J.B., "A model of flow-induced instabilities of mucus." *American Physical Society, Division of Fluid Dynamics, 48th Annual Meeting*, Irvine, CA, November, 1995.

Moriarty, J.A. and Grotberg, J.B., "A model of flow-induced instabilities of mucus." *Biomedical Engineering Society Annual Fall Meeting*, Boston, MA, October 1995.

Capillary-Elastic Instabilities in Microgravity

PRINCIPAL INVESTIGATOR: Prof. James B. Grotberg

Northwestern University

CO-INVESTIGATORS:

Halpern, D.

University of Alabama, Tuscaloosa, AL

Task Objective:

The research proposed in this application addresses the capillary-elastic instabilities of liquid-lined flexible tubes in the presence of variable surface tension and imposed perturbations. Three important microgravity applications of this fundamental problem are (i) closure and reopening of small airways in the lung, (ii) annular extrusion processes, and (iii) two-phase flow in porous and poro-elastic materials.

Task Description:

The proposed work includes both theoretical and experimental investigations. The investigators will explore the possible stabilization of this system by imposing forced oscillation, either of the tube geometry (radius or length) or of interfacial stress from oscillating the core fluid. Also the role of surfactants and surface charge in stabilization will be examined, as well as surface fluid sources/sinks and non-Newtonian properties. Benchtop experiments will be performed to simulate airway closure, post-closure filling flows, and airway reopening by using rigid and flexible tubes. Development of a set of experiments which could be performed in space is also addressed.

Task Significance:

The closure and subsequent reopening of lung airways due to capillary-elastic instabilities contributes strongly to the mechanical response of the lung during breathing. Understanding the underlying fluid mechanical phenomena is a fundamental inquiry in pulmonary physiology, both in normal and microgravity environments. Airway closure in normal gravity tends to occur in the lower lung due to its weight. In microgravity PI anticipate two important ramifications of weightlessness with regard to airway closure: (1) airway closure will be more prevalent, and (2) it will occur uniformly throughout the lung. Airway closure has been documented in microgravity during the 9-day flight of Spacelab Space Life Sciences-1. All seven crew members performed pulmonary function tests which showed that they experienced airway closure and it was more uniformly distributed. Airway closure may compromise gas exchange in astronauts, particularly during extra-vehicular activity. In a setting of more uniformly distributed closure that provides, this becomes a potentially significant issue for limited gas exchange for the astronaut.

Technologically related applications of this work are the two air-liquid surfaces in annular extrusion methods for manufacturing small hollow fibers or co-extrusion of annular fibers with a fluid core. This is an exact analogy to this research problem, and would provide an interesting range of elastic moduli to investigate in our research. The manufacturing applications often involve polymer liquids which are non-Newtonian, a feature also of the lung's liquid lining.

Among the other important engineering applications of these investigations is the development of models of two-phase flow in porous media where surface tension phenomena modify the connectivity of the fluid phases and thereby affect the overall flow behavior. This work is also related to the more general problem of interfacial flows in poro-elastic media, an important engineering and technological field.

Progress During FY 1996:

This is a new project started on August 29, 1996. The progress has been aimed at writing up our experimental and theoretical results for the annular-film instabilities. The PI has a preliminary manuscript which is nearing final form. In addition, we have submitted an abstract to a national meeting (Experimental Biology '97, to be held in New Orleans in April, 1997) to present the work.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 0

PhD Students: 1

TASK INITIATION: 8/96 EXPIRATION: 8/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NAG3-195

RESPONSIBLE CENTER: LeRC

Effects of Convection on the Thermocapillary Motion of Deformable Drops

PRINCIPAL INVESTIGATOR: Prof. Hossein Haj-Hariri

University of Virginia

CO-INVESTIGATORS:

Borhan, A.

Pennsylvania State University

Task Objective:

The objective of this theoretical effort is to extend the understanding of thermocapillary motion of drops by including drop deformations. The convective transport of momentum and energy as well as the effects of container walls will be accounted for by the work.

Task Description:

The focus of the initial effort is on the following tasks (a) theoretical work on the boundary-integral formulation for the axi-symmetric motion and deformation of a drop in a cylindrical container, (b) finite-volume formulation of the same problem using domain-mapping techniques, and (c) analysis of the transport of a color function to demarcate the drop boundary.

Task Significance:

This research will provide information on the motion and shapes of drops driven by interfacial tension gradients. A novel feature of this research is that to facilitate the modeling of this phenomenon using a computer, the sharp boundary between the drop and the surrounding liquid is "smeared" in the computations. The anticipated outcome of this research is the speed and shapes of the drops under various conditions and an enhanced understanding of how much the interface can be smeared before the results are intolerably degraded.

Progress During FY 1996:

A parametric study of the effect of moderate convection of momentum and energy on the thermocapillary migration of a single drop has been completed. It is found that interfacial deformations arising from the convection of energy at small Reynolds numbers are negligible. The convection of energy does retard the thermocapillary motion of gas bubbles and viscous drops. On the other hand, though inertial effects cause slight deformations, they have a pronounced effect in retarding the drop's motion. Inertial effects tend to have a weaker influence on the motion of viscous drops compared to gas bubbles. The direction of elongation of the drop depends on the density ratio between the two phases.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 3

TASK INITIATION: 12/92 EXPIRATION: 11/95

PROJECT IDENTIFICATION: 962-24-05-45

NASA CONTRACT No.: NAG3-139

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Nadim, A., Borhan, A., and Haj-Hariri, H., Tangential stress and Marangoni effects at a fluid-fluid interface in a Hele-Shaw cell. *J. Coll. Interface Sci.*, vol. 181, pp. 159 - 164 (1996).

Proceedings

Haj-Hariri, H. and Borhan, A., "Thermocapillary motion of deformable drops in the presence of surface contamination." Proceedings of the 18th Boundary Element Int. Conf., Brago, Portugal, September, 1996.

Haj-Hariri, H. and Borhan, A., "Time-dependent thermally-driven interfacial flows in multilayered fluid structures." Proceedings of the Third Microgravity Fluid Phys. Conf., NASA Lewis, Cleveland, OH, June 1996.

Instability Mechanisms in Thermally-Driven Interfacial Flows in Liquid-Encapsulated Crystal Growth

PRINCIPAL INVESTIGATOR: Prof. Hossein Haj-Hariri

University of Virginia

CO-INVESTIGATORS:

Borhan, A.

Pennsylvania State University

Task Objective:

The objective of this program is to perform a comprehensive analytical and numerical study of the stability of thermally-driven interfacial (thermocapillary) flows in layered fluid structures, in order to develop a better understanding of the influence of multiple, deformable fluid-fluid interfaces on the nature of time-dependent flows in thermocapillary-driven multi-layered fluid structures.

Task Description:

This investigation extends previous preliminary studies of thermally-driven convection in multilayered fluid structures by considering the effects of fluid-fluid interface deformations on the structure of the basic flow state in these systems, as well as the stability of the resulting steady flow in each layer. Multi-layered structures in the differentially heated rectangular cavity with a free surface will be investigated first. An extension of a numerical method developed as part of our recent NASA Fluid Physics grant will be used to account for finite deformations of the fluid-fluid interfaces, as well as the liquid-solid interactions. The stability of the computed base state flows will be examined by performing linear stability analyses in the model problem, and the critical parameters affecting the stability of these systems will be identified.

Task Significance:

Thermocapillary flows are of considerable technological importance in materials processing applications such as crystal growth from the melt, particularly under microgravity conditions. The electronic properties of the solidified material in this process can be critically affected by the structure of the thermocapillary flow, particularly time-dependent flow, induced in the melt. Hence, the structure and stability of thermocapillary convection has been a subject of active research in an effort to better understand, and eventually control, thermally-induced motions in the melt and optimize the quality of the resulting product. When the melt contains a volatile component, the need for stringent control of the melt stoichiometry during processing is another important consideration. Encapsulation of the melt by another liquid layer has been developed as a means of controlling the stoichiometry. However, the addition of the new interface between the melt and the encapsulant can lead to interesting new dynamics, including instabilities, which have not been explored yet.

The results of the proposed study will enhance our understanding of the structure of thermally-driven flows in multi-layered structures by quantifying the influence of finite interface deformations, and will lead to improved physical insight into the role of interactions among multiple fluid-fluid interfaces in determining the stability characteristics of flows driven by interfacial tension gradients. Though not directly applicable to crystal growth processes of practical interest, a better understanding of these model problems serves to identify the instability mechanisms that are responsible for the experimentally observed instabilities, and suggest possible steps for minimizing, and eventually controlling, such instabilities.

Progress During FY 1996:

This is a new project which is just getting started.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/96 EXPIRATION: 7/97

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-191

RESPONSIBLE CENTER: LeRC

Evaporation from a Meniscus within a Capillary Tube in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Kevin P. Hallinan

University of Dayton

CO-INVESTIGATORS:

Ervin, J.

University of Dayton

Task Objective:

The primary objectives of this project are to perform (i) macroscopic studies of evaporation from a capillary meniscus, (ii) preliminary measurements of the flow field in the evaporating thin film region, and (iii) further development of the Coherent Forward Scattering Particle Image Velocimetry (CFSPIV) technique applied to the evaporating thin film region near the contact line.

Task Description:

This is a proposal for a fundamental study in microgravity of evaporation from curved liquid-vapor interfaces in capillaries in the interfacial region controlled: (i) by surface tension; and by (ii) surface forces due to solid-liquid intermolecular interactions. The experiments will include simultaneous particle image velocimetry (PIV), interferometry, and wall temperature measurement in order to obtain fluid velocities, interface shape, and wall temperature in the thin film region. Thermocapillary effects will be quantified by the measured wall temperature and the fluid velocity profile of the near contact line region of a heated and evaporating meniscus in the thin film region.

Task Significance:

The study of the thermocapillary effect on the interfacial instability of an evaporating extended meniscus may help explain the failure of the Capillary Pump Loop in a microgravity environment. The knowledge obtained from this study could result in radical new heat exchanger technologies that will benefit both space exploration and terrestrial applications.

Progress During FY 1996:

Work has been completed on the macroscopic studies of evaporation from a heated capillary meniscus. This work has focused on: evaluating the effectiveness of heat transport from the whole of evaporating meniscus; investigating the stability of the heated and evaporating meniscus and attempting to gain an improved understanding of the mechanisms leading to the instabilities; and finally on attempting to improve the heat transfer effectiveness and interfacial stability through the use of either surface coating on the capillary wall or the addition of a non-volatile solute to the solvent. The progress has continued toward the development of the CFSPIV technique to the heated evaporating near contact line region. The configuration of an interferometric metrology set-up to measure the displacement of the microscope stage to the fixed objective lens to an accuracy of 0.05 microns. The production of calibration diffraction image of the light scattered by 0.2 - 3.2 microns PMMA particles in methanol for particle positions ranging in distance from the focal plane of the imaging lens of -50 microns to 50 microns was completed. A correlations technique to compare actual particle images individually to a bank of calibration images to determine the position of the particles relative to the lens focal plane was completed.

The CFSPIV technique has been applied to the near contact line region of a heated and evaporating meniscus along an inclined flat plane. It has been used for the first time to measure the velocity field very close to the contact line, where the film thickness is less than 100 microns. Spatial resolution in locating particles within the film has been shown to less than a fraction of a micron in all directions. Accuracies of the measured velocity components have been estimated to be less than 3% full scale.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	3	BS Degrees:	3
MS Students:	0	MS Degrees:	0
PhD Students:	3	PhD Degrees:	2

TASK INITIATION: 12/94 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 963-25-0A-21

NASA CONTRACT NO.: NAG3-139

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Brown, J.R. and Hallinan, K.P., Effects of heat induced instabilities on the heat transfer of a stably evaporating meniscus. AIAA, 96-0723, (1996).

Presentations

He, Q., Hallinan, K.P., "The development of a full field three-dimensional microscale flow measurement technique for application to near contact line flows." presented at the 3rd Microgravity Fluids Conference, Cleveland, OH, June 13-15, 1996.

He, Q., Hallinan, K.P., and Ovryn, B., "3-d full field PIV with pattern recognition applied to thin liquid films." Presented at the Optical Society of America Annual Meeting, Portland, OH, October 1995.

Prat, D.M. and Hallinan, K.P., "The effects of near contact line thermocapillary stresses on the wetting characteristics of a heated, evaporating meniscus within a capillary pore." Presented at the National Heat Transfer Conference, Houston, TX, August 5-9, 1996.

A Study of the Microscale Fluid Physics in the near Contact Line Region of an Evaporating Capillary Meniscus

PRINCIPAL INVESTIGATOR: Prof. Kevin P. Hallinan

University of Dayton

CO-INVESTIGATORS:

Ovryn, B.
Allen, J.NYMA, Inc.
University of Dayton

Task Objective:

The primary objectives of this project are to perform (i) macroscopic studies of evaporation from a capillary meniscus, (ii) preliminary measurements of the flow field in the evaporating thin film region, and (iii) further development of the Coherent Forward Scattering Particle Image Velocimetry (CFSPIV) technique applied to the evaporating thin film region near the contact line.

Task Description:

This is a proposal for a fundamental study in microgravity of evaporation from curved liquid-vapor interfaces in capillaries in the interfacial region controlled: (i) by surface tension; and by (ii) surface forces due to solid-liquid intermolecular interactions. The experiments will include simultaneous particle image velocimetry (PIV), interferometry, and wall temperature measurement in order to obtain fluid velocities, interface shape, and wall temperature in the thin film region. Thermocapillary effects will be quantified by the measured wall temperature and the fluid velocity profile of the near contact line region of a heated and evaporating meniscus in the thin film region.

Task Significance:

The study of the thermocapillary effect on the interfacial instability of an evaporating extended meniscus may help explain the failure of Capillary Pump Loop in a microgravity environment. The knowledge obtained from this study could result in radical new heat exchanger technologies that will benefit both space exploration and terrestrial applications.

Progress During FY 1996:

This is a new grant just started in May 1997. The PI is now in the process to observe the wettability changes of a heated and evaporating meniscus in a slotted capillary channel.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/96 EXPIRATION: 7/98

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-191

RESPONSIBLE CENTER: LeRC

Interfacial Transport and Micellar Solubilization Processes

PRINCIPAL INVESTIGATOR: Prof. T. A. Hatton

Massachusetts Institute of Technology (MIT)

CO-INVESTIGATORS:

Smith, K.A.

Massachusetts Institute of Technology (MIT)

Task Objective:

The objective of this research is to develop and implement a new diffusion cell for the fundamental investigation of the effects of surfactants on the interfacial transport of solutes between two phases. The rates of solubilization of proteins and low molecular weight fluorophores at the interface by reversed micelles have been investigated. These are affected by the prevailing solution conditions. To date, this type of study has been hindered because the techniques used for measurement of interfacial transport processes are prone to artifacts associated with ill-defined hydrodynamic conditions. The new diffusion cell approach avoids these complications in the analysis of mass transfer results.

Task Description:

During this task period, we have concentrated on developing a new diffusion cell approach for the measurement of interfacial transport and solubilization rates without introducing hydrodynamic effects that can complicate data interpretation and analysis. The technique relies on the fact that many fluorophores can be bleached irreversibly when exposed to high intensity light sources for brief periods of time. The rate at which fluorescence is recovered in the bleached zone depends on the diffusion of fluorophores from outside this region. Our task has been to set up the equipment, to integrate the various components, and to establish a methodology for data analysis. The solubilization rates of a number of proteins and low molecular weight fluorophores have been investigated over a range of solution conditions. A testing program to identify the important parameters ranges over which a space-based experimental study would be beneficial was undertaken.

Task Significance:

Interfacial transport and solubilization processes are important in many industrial, commercial and home operations, ranging from large-scale reaction and separation processes to detergency in dishwashing and laundry applications. New separation and reaction technologies based on surfactant self-assembly show promise for reducing the potential for environmental contamination in many industrial processes, or for remediation of already contaminated resources. Through the development of techniques to measure the rates at which the processes of interest occur, and relating these data to the chemical properties of the systems under study, we will be in a position to design more effectively the surfactants for specific new applications. In some cases, gravity-driven convective currents will complicate the data analysis and interpretation, and this establishes the need to conduct experiments under the low-gravity conditions of a space-based experimental program.

Progress During FY 1996:

Optimization of the FRAP system operating parameters has been carried out. To obtain acceptable levels of sensitivity, a minimum photobleaching extent of 30% is required to perturb the system sufficiently. This level of energy input into the system requires very low fluorophore concentrations, on the order of 100 nM. A video detection system of increased sensitivity has been set up to allow observation of dilute solutions. In addition, a mechanism has been devised to shield the test cell from the observation beam except at data-acquisition times to allow increases in the observation beam strength. A translation stage now permits scanning of the photobleaching beam across the sample cell parallel to the interface, allowing greater flexibility in the bleaching pattern and effectively reducing the diffusion problem to one dimension. Finally, the entire system has been automated to facilitate multi-user operation. The solubilization rates of a range of fluorescently-labeled proteins and fluorophores have been determined in a water/reversed-micellar two-phase system have been determined over a range of pH and salt strengths in the supporting aqueous phase. The effects of solution conditions and protein size have been analyzed, and demonstrate the increased resistance to interfacial transport experienced as the protein becomes more negatively charged because of pH changes, or as the reversed micelles become smaller as the ionic strength increases. In some cases the effect of co-surfactants having affinity for some of the proteins investigated have been studied. These data are being analyzed in terms of the fluctuation energy needed to form reversed micelles at the

interface. It has been shown that interfacial resistance to transport in aqueous two-phase polymer-based systems is sufficiently low, if it exists at all, that it cannot be detected with our system. For the most part, effects due to buoyancy driven convection have been eliminated by judicious selection of fluorophore concentration and exposure time to the laser beam, although some conditions have been identified in which a low-gravity environment would be needed to obtain reliable results.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 4/93 EXPIRATION: 4/96

PROJECT IDENTIFICATION: 962-24-08-11

NASA CONTRACT NO.: NAG8-951

RESPONSIBLE CENTER: MSFC

Critical Phenomena, Electrodynamics, and Geophysical Flows

PRINCIPAL INVESTIGATOR: Dr. John Hegseth

University of New Orleans

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The first objective of this experiment is to build an experimental system in which, in analogy to a geophysical system, a compressible fluid in a spherical annulus becomes radially stratified in density through an A. C. electric field. This apparatus consists of a spherical capacitor filled with critical fluid in a temperature controlled environment. The second objective is to build another complementary cell, of the same geometry, which uses an incompressible fluid.

Task Description:

The critical fluid cell is made using a 3 inch diameter piece of cylindrical copper with a ≈ 2.5 cm diameter cylindrical hole milled through its center. Inside of this hole is placed a small spherical electrode. Because the electrical forces decrease as r^6 , the largest density changes should occur near the electrode where the E field gradient is largest. The small sphere is positioned in the center of the cell by using a small electrically conductive wire. The inner sphere is electrically isolated from the cell. An A.C. potential will be applied across the two. At each end of the outside cylindrical copper is two sapphire windows so that light may pass through the region near the inner sphere.

The highly compressible critical fluid is very sensitive to the presence of the gravitational body force making it impossible to create a spherically symmetric density gradient on Earth. These fluids are also sensitive to heat induced convection in 1g. In addition the high pressure of the critical fluid cell makes it more difficult to develop the mechanical and thermal forcing mechanisms. It is desirable to simplify the development of the cell by using an incompressible fluid at room temperature and pressure in a ground based study. This cell will also help to predict phenomena that will occur in a space experiment. A small incompressible fluid cell can create a large effective buoyancy force. This makes it possible to make a second parallel cell to complement and enhance the study of the critical fluid cell.

The incompressible cell uses two transparent sapphire domes coated with indium-tin-oxide to form the outer sphere of inner diameter 1.0000 inches. Concentric with the outer sphere is a 7/8 inch diameter conducting inner sphere at the center. The two sapphire domes are connected by a plexiglass ring that is attached to and immersed in a silicone oil bath held at a constant temperature. The inner sphere is connected to a hollow shaft attached to slip rings which allow the inner sphere to rotate. Wires from the slip ring go through the hollow shaft and into the interior of the inner copper sphere. Inside the inner sphere a heating resistor, a thermistor, and a ground wire are place to allow temperature control and voltage control. A high potential A.C. voltage source is attached to the outer sphere. A step motor is mechanically coupled to the inner sphere shaft to drive the inner sphere. The inner sphere assembly (slip ring/inner sphere/step motor) is stationary while the outer sphere assembly (sapphire domes/plexiglass plates/oil bath) is mounted on a 3-D translation stage. This allows the inner and outer spheres to be precisely move to adjust the concentricity.

Task Significance:

Some of the most urgent problems of social concern are related to geophysical flows. Examples of these problems are the climate change from the greenhouse effect, natural disasters from violent storms, and earthquakes resulting from mantel convection. Because of the disastrous effects that these and other geophysical phenomena have, considerable scientific resources have been devoted to these problems. Aside from their social consequences, geophysical flows are interesting in and of themselves and have been an inspiration for concepts such as deterministic chaos and of themselves and have been an inspiration for concepts such as deterministic chaos and two dimensional turbulence. Much of the information regarding geophysical flows has come from direct planetary observations and numerical models. The former is uncontrollable with many complicated factors influencing the flow. The later is remarkable in that it comes close at all to mimicking the former. We are developing a prototype

experimental system that will take full advantage of the microgravity environment to study these types of flows. The unique characteristic of this system - as compared to previous efforts is that we will create a system where a spherically symmetric density gradient is established in a compressible fluid. This will mimic the single most striking and obvious property of any geophysical flow, the radial density gradient. The results from our prototype experimental system should establish facts and phenomenon for simulators and theoreticians to explain under simplified conditions.

Progress During FY 1996:

We have constructed a preliminary incompressible fluid cell and begun testing of the density gradient by applying an electric field. We have to date found the following results: on applying 3000 volts (RMS) to the cell when the fluid is $\approx 20\text{mK}$ above the critical point (supercritical fluid), we have observed a fringe shift of $\sim 1/2$ of a wavelength. This corresponds to $\sim 0.005\%$ change in density near the electrode. This is less than we would expect in zero gravity. In $1g$ the presence of convection caused by buoyancy should decrease the density change.

We have also tested a preliminary incompressible cell without rotation and observed convection in the annulus. We are at present testing several visualization methods and refining the temperature control.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 0

TASK INITIATION: 8/94 EXPIRATION: 8/96

PROJECT IDENTIFICATION: 962-24-05-85

NASA CONTRACT No.: NAG3-165

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Hegseth, J., and Garcia, L., "A geophysical flow experiment in a compressible critical fluid." Proceedings of the Third Microgravity Fluid Physics Conference, NASA-LeRC, June 13-15, 1996.

A Geophysical Flow Experiment in a Compressible Critical Fluid

PRINCIPAL INVESTIGATOR: Dr. John Hegseth

University of New Orleans

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

There are two objectives. One objective is to design and construct small spherical capacitor cells and demonstrate their quality as analog systems of the earth's geophysical flows. The second objective is to examine the hydrodynamic patterns formed when the samples are driven rotationally and with temperature gradients.

Task Description:

A few centimeter diameter spherical shell shaped sample cells are to be constructed. One cell will contain very compressible near-critical sulfur-hexafluoride. The other cell will contain an incompressible fluid.

The incompressible fluid cell will be best suited for 1-g experiments without density gradients but with central and azimuthal temperature gradients combined with sample rotation. Interferometry, Schlieren, or particle image velocimetry will be used to characterize the hydrodynamics.

An electric field will be applied to the compressible fluid to induce radial density gradients as in the atmosphere. Experiments will be conducted in low-gravity aircraft to avoid earth's gravity induced stratification. After success with establishing an atmospheric analog radial density gradient in this cell, rotation and temperature gradients will be added to force three dimensional motions.

Task Significance:

The work intends to provide a laboratory apparatus that enables the study of the earth's atmospheric hydrodynamics. An adequate laboratory apparatus has not previously existed. Having an experimental model of the atmosphere to complement the many computer models is expected to improve understanding of global weather phenomena.

Progress During FY 1996:

We have improved our critical fluid cell by adding a glass outer sphere coated with Indium Tin Oxide around the inner electrode to generate a larger electric field gradient that is spherically symmetric. We are in the process of improving the temperature control with an modified thermostat. We are building a better controlled incompressible fluid cell and developing a visualization method for the incompressible cell.

Tests show that the new spherical capacitor works well in air. A polished aluminum inner sphere for the incompressible cell makes Schlieren visualization a good candidate for visualizing the incompressible flows.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 2

TASK INITIATION: 7/96 EXPIRATION: 7/98

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-191

RESPONSIBLE CENTER: LeRC

Experimental Investigation of Pool Boiling Heat Transfer Enhancement in Microgravity in the Presence of Electric Fields

PRINCIPAL INVESTIGATOR: Dr. Cila Herman

Johns Hopkins University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

In nucleate boiling regime, high heat fluxes can be achieved at relatively low superheats. Therefore, pool boiling heat transfer is important in the development of efficient cooling schemes in microgravity applications. The objective of the task is to better understand the physics of pool boiling under the influence of electric and magnetic fields, bubble cloud formation, its dynamics and the interactions of bubbles with the thermal boundary layer. Understanding these aspects of the pool boiling will help achieve improved control over bubble detachment and enhancement of heat transfer in the low gravity environment by exposing the boiling liquid to electric fields.

Task Description:

A combined multidisciplinary theoretical and experimental approach will be taken to study the heat transfer enhancement in boiling under microgravity. The experimental investigation will focus on:

- The behavior of a single vapor bubble, its dynamics and interaction with the thermal boundary layer under various E field configurations
- Boiling from several artificially generated nucleation sites and bubble interactions under the influence of E fields
- Boiling on real commercial surfaces under the influence of electric fields
- Visualization methods will be used to analyze the effects of field lines shape and distribution and field magnitude on bubble size on detachment, bubble shape and frequency, bubble motion and velocity. Holographic interferometry allows insight into the unsteady temperature fields in the liquid phase and into the complex structure of flow fields in the vicinity of bubbles.
- Results obtained from the study of the behavior of single and special configuration bubble clusters will be compared with results of numerical simulations which will be performed at the Pennsylvania State University.

Task Significance:

Results of the investigations of simple and augmented boiling surfaces will provide valuable insights for the design of phase change equipment for microgravity applications. Understanding of the mechanisms that affect the heat transfer is crucial for industrial applications where pool boiling is needed. The effects of introducing the electric field on heat transfer is also crucial from an industrial stand point. In specific, this research will help answer several issues related to pool boiling in microgravity. Example of these is the issue of whether strong electric fields can prevent coalescence of bubbles, and whether the applied fields can control the bubble diameter on detachment.

Progress During FY 1996:

The grant was awarded in late March 1996. During the first few months the work focused on two major areas:

1. Design of the Experimental Set up for visualization experiment

Under this area the following issues were addressed:

- 1.a Selection of the working fluid which has to satisfy important thermophysical and chemical properties such as
- (I) Boiling point being above the ambient temperature
 - (II) High thermal conductivity
 - (III) High heat capacity
 - (IV) Non Flammable fluid
 - (V) Non-Toxic and environmentally safe fluids

1.b The optical requirements as applied to the fluid such as transparency of the fluid and the suitability of its index of refraction for interferometric experiments

1.c The electrical properties of the fluids such as the dielectric constant and relaxation time of electric charges.

1.d The theory of bubble formation was studied as well as designs of nozzles and orifices through which the dispersed phase is injected and bubbles are formed.

1.e Conceptual design of the experimental cell allowing visualization experiments by holographic interferometry was developed.

2. Measurement of the temperature distribution around a bubble

The work here focused on developing algorithms for relating the refractive index of the fluid to the temperature of the refrigerant used in the experimental study, and on the determination of the temperature distribution around the bubble.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 3/96 EXPIRATION: 3/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-181

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Herman, C., "Experimental investigation of pool boiling heat transfer enhancement in the presence of electric fields." Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, Ohio, June 13-15, 1996.

Presentations

Herman, C., "Experimental investigation of pool boiling heat transfer enhancement in the presence of electric fields." presented at the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, Ohio, June 13-15, 1996.

Nonlinear, Resonance-Controlled Bifurcation Structure of Oscillating Bubbles

PRINCIPAL INVESTIGATOR: Dr. R G. Holt

Boston University

CO-INVESTIGATORS:

Gaitan, D.F.

Jet Propulsion Laboratory (JPL)

Task Objective:

The topic of the proposed investigation is the nonlinear dynamics of acoustically forced bubble oscillations. Specifically, the interplay between the nonlinear resonances of the system and the asymmetry imposed by 1g levitation forces required to isolate a bubble for ground-based experimentation will be investigated. The objectives of the proposed experiments are:

- 1) to observe the possible resonance-governed bifurcations by varying (within the limits imposed by 1g) the relevant parameters (driving pressure P , driving frequency f_d , equilibrium bubble radius R_0). These would be the first measurements of location and type of bifurcation ever. The expected bifurcations are saddle-node, period-doubling, Faraday (Hopf-like) and Hopf; and
- 2) to identify the (P, f_d, R_0) regime where only mg experiments can obtain data, and to place bounds on the effect of the buoyant force on the threshold (P, f_d) values for each R_0 -dependent modal resonance bifurcation measured in 1g.

Task Description:

Single-bubble experiments in water at 1g with a sinusoidally-varying acoustic pressure are planned. Both acoustic levitation and optical levitation will be used to position the bubbles. Data acquisition will be accomplished via optical Mie scattering (for radius and frequency information) and high-speed video (for shape mode data).

R_0 will be varied via controlled rectified diffusion between 0.2 and 2. (normalized to the linear monopole resonant size of a bubble with fixed f_d). P will be varied between 0.05 and 1.5 atm for the acoustic levitation experiments. f_d will be varied between 0.2 and 2.5 (normalized to the linear resonance frequency of a bubble of fixed R_0).

The roles of surface tension, viscosity and especially surface viscosity in determining the location in parameter space where the shape bifurcations take place will be examined by varying the type and concentration of added surfactant to the host liquid, usually water. It should be possible to increase the value of P where the Faraday instability sets in, perhaps "uncovering" some of the predicted saddle-node/period-doubling bifurcations for purely spherical motion even in 1g.

Task Significance:

As a brief introduction, consider the complicated nature of fixed-parameter driven oscillations of a bubble in water. Experimental observations of single-bubble oscillations have yielded a wide variety of phenomena: periodic and period-doubled spherical oscillations [Holt, R. Glynn and Lawrence A. Crum, J. Acoust. Soc. Am. 91, 1924 (1992)]; periodic, quasiperiodic and chaotic multi-mode shape oscillations [Holt, R.G., Proceedings of the 13th International Congress on Acoustics, Belgrade, Yugoslavia, P. Pravica and G. Drakulic, eds., (Sava Centar, Belgrade, 1989), Volume 1, p. 131]; and, most recently, periodic, period-doubled, quasiperiodic and chaotic sonoluminescence! [Holt, R.G., D.F. Gaitan, A.A. Atchley and J. Holzfuss, Phys. Rev. Lett. 72, 1376 (1994)]. Despite this seeming wealth of information, there is still no global 'map' of the parameter space (P, f_d, R_0) which shows the possible behaviors, and the bifurcation curves which govern changes in behavior.

There are two reasons for the gap in experimental knowledge. First, prior experiments, the first of their kind, were limited in scope. Second, for 1g acoustic levitation of bubbles, the same acoustic field provides levitation (positioning) and drives the oscillations. Changing P changes the levitation position (which is displaced from the antinode due to gravity), making execution and calibration difficult.

There exists much theoretical work on the small amplitude, spherical problem, and this is largely borne out by experiment. Some spherical models have been pushed to large amplitudes, where a rich resonance-bifurcation structure is predicted, but has not been observed experimentally, largely due to the onset of stable shape oscillations through the Faraday instability.

Recently, some exciting new theoretical work had addressed the Faraday bifurcation by examining (for limited modes and frequencies only) the nonlinear resonant coupling (1:1 and 1:2 frequencies) between shape and volume modes. In particular, Yang, Feng and Leal [Yang, S.M., Feng, Z.C. and L.G. Leal, J. Fluid Mech. 247, 417 (1993)] show that the very nature of the coupling and relative mode stability are altered when there is some initial deformation due to an external flow; thus, for 1g experimentation, the observed onset and stability of shape oscillations will occur at lower pressures, and will likely show other anomalous features with respect to the ideal, purely isotropic case (which could be realized in microgravity).

Progress During FY 1996:

1g measurements are complete. Measurements of the onset conditions of shape oscillations on bubbles from 1 to 110 microns in radius have been performed at a constant frequency (20.6 kHz) in pure water as a function of acoustic pressure and dissolved gas concentration. Oscillation amplitude prior to onset, acoustic pressure, mode, equilibrium size and oscillatory radius were recorded at the instant of transition to shape oscillation for all bubbles. Preliminary analysis has yielded many results, including observation of anomalous dynamic mass transport stability for very small bubbles. Analysis indicates that a classification scheme involving external and internal resonances can organize and predict the bifurcation behavior observed. Analysis is still underway, and the first of many publications are now appearing, see Bibliography section following.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/94 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 962-24-04-15

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Holt, R.G., and Gaitan, F.D. Observation of stability boundaries in the parameter space of single bubble sonoluminescence. Phys. Rev. Lett., (October 1996).

Proceedings

Holt, R.G., and Gaitan, D.F. "Proceedings of the 3rd Microgravity Fluid Physics Conference, Cleveland, OH, 1996, NASA CP 3338, p. 591." Proceedings of the 3rd Microgravity Fluid Physics.

Presentations

Gaitan, D.F., and Holt, R.G. "Observation of mass transport stability and Faraday instability: why stable single bubble sonoluminescence is possible." 3rd joint meeting of the Acoustical Society of America and the Acoustical Society of Japan, Honolulu, HI, 1996.

Holt, R.G., and Gaitan, D.F. "Single Bubble Sonoluminescence: Illuminating anomalous bubble mechanics." 49th meeting of the American Physical Society, Division of Fluid Dynamics, Syracuse, NY, 1996.

Thermocapillary Instabilities and g-jitter Convection

PRINCIPAL INVESTIGATOR: Prof. George M. Homsy

Stanford University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objectives of this study are: (i) To study the time dependent flows that result from transient accelerations present aboard orbiting spacecraft; and (ii) To study both experimentally and theoretically the types of complex flows that can result from surface tension gradients in fluids.

Task Description:

The study of so-called g-jitter effects seeks to understand the effect of transient accelerations on fluid motion. One of the main ways in which g-jitter can cause significant fluid motion is through the coupling of accelerations to resonant modes within the fluid. In this way, small dynamic forcing due to jitter can have large effects on the fluid state. Our studies in this area involve the use of numerical and analytic models to find parallel flow solutions for both buoyancy and thermocapillary driven convection, and to analyze their stability with respect to more complex flows.

The study of thermocapillary convection involves the understanding of the flows that arise when there is a combination of a free surface and a temperature variation along it. Such a situation sets up a surface tension gradient in the interface that can drive a flow that may be quite vigorous and complex in either time or space. Our experimental work has involved probing the dynamics of such flows in a range of parameters for which we are particularly interested in combinations of container size, fluid properties (Prandtl number) and applied temperature driving (Marangoni number) that involve multiple modes becoming unstable simultaneously, opening up the possibility of complex dynamics leading to thermally induced turbulence.

Task Significance:

The study of the behavior of fluid behavior in microgravity conditions is important for both scientific and technological reasons, since there are both life support systems and scientific experiments that involve the fluid state of matter. The results from this work will enhance our understanding of how the basic forces acting upon fluids in the microgravity environment cause a variety of responses. Such an understanding will contribute to better fluid handling / management techniques and may suggest some innovative processes for improved fluids management. In addition, the basic understanding achieved will have impact on the planning and interpretation of a wide range of scientific experiments in materials processing, biotechnology, and other fields involving materials in the fluid state.

Progress During FY 1996:

Much of our progress has been documented in published papers in the literature, given in the bibliography.

In the area of g-jitter convection, we have examined the question of the response of a heated fluid when subjected to simple harmonic oscillations in the body force. We find that under conditions where the frequency and amplitude of oscillation is near a normal mode of the fluid, small driving in the form of g-jitter can result in a large fluid response associated with parametric resonance. When we analyze the response above the point of resonance, we find the very surprising result that the response is a nonlinear oscillation of the fluid as a whole, with transient turbulent bursts of secondary motion superposed.

We have recently begun to analyze what happens when the underlying motion is driven by thermocapillarity rather than buoyancy, and how the g-jitter can couple to thermocapillary modes. Surprisingly, we have discovered a set of parallel flow solutions - analogous to those in parallel flow solutions exist for arbitrary orientation of the jitter relative to the mean temperature gradient driving the motion. Work is now in progress to compute some of these parallel flows, and to study their stability properties.

In the area of our experimental studies of thermocapillary convection, we have successfully redesigned the test cell to allow a more flexible choice of cell aspect ratios to be studied and have significantly improved our flow visualization and velocimetry (reference 4). Our initial studies discovered an interaction between the first mode of instability - a steady three dimensional convection - and a relaxation oscillation associated with convection in the meniscus region of the fluid. By suitable variation of cell aspect ratio, it is possible to 'tune' the geometry so that both two and three dimensional modes become unstable simultaneously. Current work is devoted to exploring this case to can result. In addition, we are currently investigating the possibility of real time imaging of the thermal field using thermally sensitive dyes in order to complement the information on flow fields.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 4/93 EXPIRATION: 4/96

PROJECT IDENTIFICATION: 962-24-05-48

NASA CONTRACT No.: NAG3-147

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Braunsfurth, M. and Homsy, G.M., Combined thermocapillary-buoyancy convection in a cavity: an experimental study: Part II. Phys. Fluids, (1996).

Farooq, A. and Homsy, G.M., Linear and nonlinear dynamics of a differentially heated slot under gravity modulation. J. Fluid Mech., vol.313, pp. 1-38 (1996).

Gillon, P. and Homsy, G.M., Combined thermocapillary-buoyancy convection in a cavity: an experimental study. Phys. Fluids, (1996).

Proceedings

Braunsfurth, M. and Homsy, G.M., "Experimental Study of Buoyant-Thermocapillary Convection in a Rectangular Cavity." Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June, 1996.

Presentations

Braunsfurth, M. and Homsy, G.M., "Combined thermocapillary-buoyancy convection in a in a cavity: an experimental study." American Physical Soc. Meeting, Div. Fluid Dynamics, Irvine CA, November 1995.

Braunsfurth, M., and Homsy, G.M., "Combined thermocapillary-buoyancy convection in a cavity: an experimental study." Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 1996.

Problems in Microgravity Fluid Mechanics: Thermocapillary Instabilities and G-Jitter Convection

PRINCIPAL INVESTIGATOR: Prof. George M. Homsy

Stanford University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objectives of this study are: (i) To study the time dependent flows that result from transient accelerations present aboard orbiting spacecraft; and (ii) To study both experimentally and theoretically the types of complex flows that can result from surface tension gradients in fluids.

Task Description:

The study of so-called g-jitter effects seeks to understand the effect of transient accelerations on fluid motion. One of the main ways in which g-jitter can cause significant fluid motion is through the coupling of accelerations to resonant modes within the fluid. In this way, small dynamic forcing due to jitter can have large effects on the fluid state. Our studies in this area involve the use of numerical and analytic models to find parallel flow solutions for both buoyancy and thermocapillary driven convection, and to analyze their stability with respect to more complex flows.

The study of thermocapillary convection involves the understanding of the flows that arise when there is a combination of a free surface and a temperature variation along it. Such a situation sets up a surface tension gradient in the interface that can drive a flow that may be quite vigorous and complex in either time or space. Our experimental work has involved probing the dynamics of such flows in a range of parameters for which we are particularly interested in combinations of container size, fluid properties (Prandtl number) and applied temperature driving (Marangoni number) that involve multiple modes becoming unstable simultaneously, opening up the possibility of complex dynamics leading to thermally induced turbulence.

Task Significance:

The study of the behavior of fluid behavior in microgravity conditions is important for both scientific and technological reasons, since there are both life support systems and scientific experiments that involve the fluid state of matter. The results from this work will enhance our understanding of how the basic forces acting upon fluids in the microgravity environment cause a variety of responses. Such an understanding will contribute to better fluid handling / management techniques and may suggest some innovative processes for improved fluids management. In addition, the basic understanding achieved will have impact on the planning and interpretation of a wide range of scientific experiments in materials processing, biotechnology, and other fields involving materials in the fluid state.

Progress During FY 1996:

This is a new project which just started in September 1996.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 9/96 EXPIRATION: 8/97

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-147

RESPONSIBLE CENTER: LeRC

Turbidity of a Binary Mixture Very Close to the Critical Point

PRINCIPAL INVESTIGATOR: Prof. Donald T. Jacobs

The College of Wooster

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This experimental activity is intended to measure the temperature dependence of light transmitted through a density matched, fluid mixture's near critical, consolute point.

Task Description:

1. Develop a room temperature thermal control system for the sample that enables temperature control inside of ± 3 microK;
2. Assemble and use phase sensitive detection system to detect the small light intensity variations expected close to the consolute point;
3. The turbidity data will be reduced according to the formalism of Puglielli and Ford (Phys. Rev. Lett. 25, 243 (1970)) and of R.A. Ferrell (Physica A 177, 201 (1991)).
4. Undergraduate students will assist Prof. Jacobs, making his activity a strong educational experience for the students.

Task Significance:

The resulting data will be used to confirm and quantify a small exponent " η " in the denominator of $\{(1+q\chi)^{2-\eta}\}$ that describes the correlation length dependent distribution of scattered light from near critical fluids. Also, "two-scale universality" can be tested from the data set when combined with measurements of the heat capacity.

Progress During FY 1996:

Preliminary data were taken on two samples of the fluid mixture Methanol-Cyclohexane. The first sample had a thin (1.6 mm) optical path length with bulk fluids surrounding. This sample was not a critical concentration (excess cyclohexane) and critical-point wetting resulted in fluid bubbles forming on the windows and growing in size as a function of temperature. While some measurements were made to characterize this unexpected behavior, a different sample and cell geometry were used to proceed with the intended experiment.

In order to avoid the mixing problems also encountered in the thin cell geometry, our next cell used a uniform fluid thickness of 10.8 mm to investigate a critical composition sample. We also used a small stir bar to mix the fluids when the temperature was changed. This sample gives very consistent data that reproduces, yet is more precise than, that reported in the literature. We were able to approach the critical point to within 10ppm in reduced temperature, which is well on the way to the needed 0.1ppm approach. Additional time and replacement of a few key instruments will be necessary to achieve the data that can determine the exponent h .

Four more students have received their Bachelors degrees and new students have been brought into the learning experience. One student (Chris Ditchman) was selected for a Barry M. Goldwater Scholarship.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	14	BS Degrees:	9
MS Students:	0	MS Degrees:	0
PhD Students:	0	PhD Degrees:	0

TASK INITIATION: 1/93 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-24-05-74

NASA CONTRACT NO.: NAG3-140

RESPONSIBLE CENTER: LeRC

Kinetic and Transport Phenomena in a Microgravity Environment

PRINCIPAL INVESTIGATOR: Prof. David Jasnow

University of Pittsburgh

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Theoretical research will be carried out in several areas which involve kinetic and transport phenomena in a microgravity environment. Specifically, attention will be paid to a number of two-phase phenomena in which thermocapillarity effects play an important role. These include, kinetics of phase separation, coupled diffusing fields (e.g., temperature and concentration) and the motion of and transport through two-phase interfaces.

Task Description:

Methods proposed include modeling of conserved order parameter dynamics in two-phase situations at the coarse grained or semimicroscopic level. Optimized codes are being developed to carry out the modeling. Coupling of order parameter to hydrodynamic fields and temperature fields are included. Thermocapillary effects such as thermomigration of drops and coalescence are observed, characterized and the underlying physics analyzed. Modeling will also be performed using techniques developed in the study of dynamical systems.

Task Significance:

The modeling at the coarse grained, semimicroscopic level allows description of phenomena over length scales ranging from the correlation length on up to semi macroscopic sizes. Local thermodynamics is included using the coarse grained free energy. The interface motion is naturally tracked and surface tension dependence on temperature and other parameters is naturally included in the specification of the coarse grained free energy. Hence universal features of transport in complex situations can be extracted, and, for example, examination of phenomenological boundary conditions can be performed at a somewhat more microscopic level.

Modeling from the perspective of dynamical maps abandons the familiar partial differential equations of the subject, but preserves the essential physics, symetries, etc. Here, if successful, a substantial improvement in computational efficiency can be achieved, at the cost of being able to compute specific material-dependent quantities.

The coarse grained modeling allows one to study phenomena from rather short length scales, i.e., on the scale of the diffuse interface thickness on up to macroscopic, the Lattice Boltzmann modeling of flows combined with parallel processing will yield efficiencies far beyond that of traditional computational fluid mechanics, and our studies of phase asymmetry indicate that a temperature gradient could be used as a control parameter in separating phases.

Progress During FY 1996:

The main effort under this theoretical project during this period has been to observe thermocapillarity effects such as thermomigration in two-phase systems, within a coarse-grained, semimicroscopic description, to characterize the phenomena and to understand the physical mechanisms for them. There are three main areas of progress: (a) The response and dynamics of a two-phase interface, in a coarse grained description, to a temperature gradient: (b) Thermomigration phenomena and phase separation kinetics in a temperature gradient, where the dominant effects are diffusion driven; and (c) A study of two-dimensional capilarity driven motion of single and multiple droplets, and phase separation kinetics, including hydrodynamical effects.

Project (a) was designed to gain insight to the effect of a temperature gradient on a two-phase interface. Both using analytic approaches and numerical relaxation methods for the dynamics of a nonconserved order parameter, we have determined the motion of an interface for a nonconserved order parameter under a temperature gradient, and have analyzed the free energy landscape for an interface under different boundary conditions.

In (b) we observe, and analyze using arguments derivable from the coarse-grained free energy for the system, thermomigration phenomena in purely diffusive systems. Temperature variations of the interfacial free energy drive

the motion, which occurs via diffusion. We have also considered phase separation phenomena in a temperature gradient to investigate potential anisotropy in domain growth introduced by the gradient.

In (c) we have developed a new method for forward integrating the coupled dynamical equations for a conserved order parameter (at the coarse grained, semimicroscopic level) and hydrodynamic flow fields for two-phase systems in two dimensions using a biharmonic solver. The method has been tested on single drop thermomigration in a temperature gradient, simple multiple drop configurations, coalescence, and phase separation kinetics.

Recent studies indicate that our research will continue on modeling multi-phase flows using coarse grained free energetics and the associated fluid mechanics equations as well as using lattice Boltzmann techniques. In the latter case very efficient codes for parallel processing are being developed for T3D processors and applied at the Pittsburgh Supercomputing Center. Research will also continue on phase asymmetry and on the development of interface equations to describe interface motions at the macroscopic level. In addition, an experimental group has begun careful experiments based on the ideas concerning the effect of phase symmetry.

In 1996, research continued on the derivation of macroscopic interface equations in two-phase incompressible fluids driven by a temperature gradient. the starting point for the derivation is a coarse-grained or mesoscopic free energy functional which goes beyond local thermodynamics via the inclusion of gradients of the order parameter (local concentration). Such a description naturally has diffuse interfaces and built in interfacial free energy related to various parameters of the model. New results involve mesoscopic corrections (i.e., corrections due to finite interface diffuseness) to the interface equations.

A second area of research begun in 1996 involves the new area of flowing thin films. We have the advantage of having some of the seminal experiments in this area done by Profs. X-l. Wu and W.I. Goldburg in this department. The materials involve complex fluids. A beginning student has undertaken an analysis of potential instabilities in a sheared liquid crystal film. This research is in its initial stages.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 1/93 EXPIRATION: 12/95
PROJECT IDENTIFICATION: 962-24-05-42
NASA CONTRACT No.: NAG3-140
RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Bhagavatula, R. and Jasnow, D., Phase asymmetry in thermocapillary motion. J. Chem. Phys., 105, 337 (1996).

Jasnow, D. and Vinals, J., Coarse-grained description of thermocapillary flow. Phys. Fluids 8, 600, (1996).

Rutgers, M.A, Wu, X-l., Bhagavatula, R., Petersen, A.A., and Goldburg, W.I., Two-dimensional velocity profiles and laminar boundary layers in flowing soap films. Phys. Fluids, (in press).

Surfactant-Based Critical Phenomena in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Eric W. Kaler

University of Delaware

CO-INVESTIGATORS:

Paulaitis, M.E.

Johns Hopkins University

Task Objective:

Our objective is to characterize by experiment and theory the kinetics of phase separation and the metastable structures formed during phase separation in a microgravity environment. We mimic microgravity using isopycnic (equal density) phases. The system we are studying is a mixture of water, nonionic CiEj ethoxylated alcohol surfactants, and near or supercritical fluids (SCF) at temperatures and pressures where the coexisting liquid phases have equal densities.

Task Description:

1. Locate and characterize ordinary critical points in surfactant / water / SCF mixtures about which two coexisting phases will be matched in density.
2. Examine using scattering methods the equilibrium structures that form in surfactant / water / SCF mixtures.
3. Examine using scattering methods the non-equilibrium structures that form inside both the binodal and spinodal regions with either temperature or pressure jumps.

Task Significance:

The potential ability to control phase separation of liquid mixtures in a microgravity environment has led us to investigate novel processing strategies for materials synthesis in space. As a cost-effective first step in this research program we have begun to examine phase separation kinetics under simulated microgravity conditions in earth-based experiments. These conditions are achieved by using mixtures of surfactants and highly compressible supercritical fluids with water to produce two coexisting liquid phases of equal density, thus eliminating the density differences that affect phase separation. Phase separation is initiated by using either temperature or pressure changes that cause the mixture to enter a metastable or unstable region. An improved basic understanding of the role of gravity in phase separation would eventually help guide experiments investigating novel processing strategies for materials synthesis in space.

Progress During FY 1996:

Our approach for locating two isopycnic phases is to first locate them in three-phase equilibrium with a gas phase. This is easier than directly locating them in a binodal because large regions of temperature and pressure space can be searched for isopycnic phases without having to change the overall composition of the sample. After locating isopycnic phases in a three-phase region, it is relatively straightforward to refine the choices of temperature, pressure and composition to locate isopycnic phases in the two-phase region that borders the three-phase triangle. These are the isopycnic phases that can then be utilized in performing phase separation kinetics experiments.

We have continued our characterization of isopycnic phases in ternary mixtures of CiEj surfactants, CO₂, and H₂O. Measured and reported density measurements together with model calculations for the mixture C₈E₅ / CO₂ / H₂O show that non-ideal mixing between CO₂ and H₂O is primarily responsible for the formation of isopycnic phases in this mixture. Other SCFs are of interest, but this work with CO₂ shows that necessary conditions for the formation of isopycnic phases are that the SCF must be denser than water and have its aqueous solubility enhanced by the presence of surfactant. Candidate supercritical fluids are the halogenated refrigerants containing at least one hydrogen.

With the approach outlined above, we have completely characterized isopycnic phases in the quaternary mixture C₁₀E₆ / trifluoromethane (R23) / H₂O / D₂O. The changes in density at different H₂O/D₂O ratios allows changes in the conditions for which two isopycnic phases are in equilibrium. We located, at 139 bar and 21 °C, the mixture

critical composition at 4.0 wt % C10E6, 2.7 wt% R23, 56.4 wt% H2O and 36.9 wt% D2O by finding the point where the phase volumes are equal. In addition, we have measured the phase boundary at a constant surfactant to water ratio to define the conditions necessary for two isopycnic phases to exist. Similar types of phase behavior characterizations have been performed to enable isopycnic phases to form both near and away from the critical point.

Some confusion exists in the literature regarding the kinetic behavior of phase separating mixtures of surfactant and water. Typically, mixtures of surfactant and water can be expected to follow universal behavior for binary mixtures, as was shown for a mixture of C₁₂E₅ and water by others. This universal behavior is described well by scaling equations. However, different groups have studied mixtures of C₁₂E₆ and brine and discovered that for relatively small quench depths, the kinetics of domain growth are described by a stretched exponential approach to a pinned domain size.

In order to verify that surfactant water mixtures behave as universal binary liquid mixtures and to develop small angle light scattering equipment for studying phase separation kinetics, a study was made of the phase separation kinetics of mixtures of C₁₂E₅ and water. Deep and shallow quenches of both critical and off-critical compositions were studied using small angle light scattering.

Samples of critical composition were quenched to depths varying from 2 mK to 29 mK from the critical temperature. When Ising model critical exponents are used for scaling, all the data collapse to a single curve that obeys universal scaling as set forth by Furukawa, and show no evidence of pinning behavior. Also, for off-critical quenches, the domains were found to grow as $t^{1/3}$, consistent with diffusion-limited Lifshitz-Slyozov-Wagner theory. We are in the process of expanding these light scattering studies to mixtures of brine / C₁₂E₆ and D₂O / C₁₂E₅.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 3

TASK INITIATION: 1/93 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-24-05-75

NASA CONTRACT NO.: NAG3-142

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Zielinski, R.G., Paulaitis, M.E., and Kaler, E.W., Isopycnic phases in supercritical fluid / water / C₁₂E₅ mixtures. J. Phys. Chem., 100, 9465 (1996).

Zielinski, R.G., Paulaitis, M.E. and Kaler, E.W., A new cell for neutron scattering at elevated pressures. Rev. Sci. Inst., 67, 2612 (1996).

Surfactant-Based Critical Phenomena in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Eric W. Kaler

University of Delaware

CO-INVESTIGATORS:

Paulaitis, M.E.

Johns Hopkins University

Task Objective:

Our objective is to characterize by experiment and theory the kinetics of phase separation and the metastable structures formed during phase separation in a microgravity environment. The system we are studying is a mixture of water, nonionic CiEj ethoxylated alcohol surfactants, and near or supercritical fluids (SCF) at temperatures and pressures where the coexisting liquid phases have equal densities (isopycnic). An improved understanding of the role gravity has in governing the kinetics of phase separation will suggest novel earth-based methods to exploit the slow phase separation in materials manufacturing. These pilot efforts would eventually be used in space on a larger variety of systems.

Task Description:

1. Locate and characterize ordinary critical and tricritical points in surfactant / water / SCF mixtures about which two coexisting phases will be matched in density.
2. Examine using scattering methods the non-equilibrium structures that form inside both the binodal and spinodal regions with either temperature or pressure jumps.
3. Identify, with the aid of engineering equations of state, polymerizable oils which form isopycnic phases.
4. Carry out a polymerization reaction in an isopycnic mixture as it is phase separating.
5. Conduct polymerization reactions in mixtures where the polymer latex has the same density as the solvent.

Task Significance:

The potential ability to control phase separation of liquid mixtures in a microgravity environment has led us to investigate novel processing strategies for materials synthesis in space. As a cost-effective first step in this research program, we have begun to examine phase separation kinetics under simulated microgravity conditions in earth-based experiments. Earth-based polymerization schemes in model isopycnic mixtures will be used in an attempt to capture some of the non-equilibrium microstructure in the mixture. An improved basic understanding of the role of gravity in phase separation and materials synthesis would eventually help guide experiments investigating novel processing strategies for materials synthesis in space.

Progress During FY 1996:

This project is a continuation of a previous grant, and was just recently funded under the new NRA. We are in the process of expanding our light scattering studies to include mixtures of brine/C₁₂E₆ and D₂O/C₁₂E₅.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 3

TASK INITIATION: 9/96 EXPIRATION: 9/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-195

RESPONSIBLE CENTER: LeRC

Bubble Generation in a Flowing Liquid Medium and Resulting Two-Phase Flow in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Yasuhiro Kamotani

Case Western Reserve University

CO-INVESTIGATORS:

Ostrach, S.
Kadambi, J.Case Western Reserve University
Case Western Reserve University

Task Objective:

The objective of this work is to study bubble generation in a liquid flow in a pipe under reduced gravity conditions. The Principal Investigator will investigate both experimentally and theoretically the bubble size and frequency of the generation and the resulting two-phase flow but it also concerns the fluid mechanical aspects of boiling in forced flow in microgravity. By injecting a gas into a liquid flow in a pipe through a small hole in the pipe wall, the Principal Investigator will investigate how the bubble expands and detaches from the wall. The Principal Investigator will also heat to simulate boiling and investigate the effect of thermocapillary flow around bubble on the bubble generation.

Task Description:

The Principle Investigator will perform 1) An experimental study of bubble generation in a liquid pipe flow with the bubble injection from a hole in the wall, 2) An experimental study of the effect thermocapillary flow on bubble generation, 3) A refinement and modification of the current theoretical model for bubble generation, and 4) A scaling analysis of the bubble generation problem including the effect of thermocapillarity.

Task Significance:

Two-phase systems including gas/liquid and liquid/liquid contacting systems are common phenomena encountered in many space applications, such as spacecraft thermal control systems, propulsion systems, power generation systems, cryogenic transfer and storage systems, life support systems, and other chemical/material process engineering systems. The design of two-phase systems for space applications requires a knowledge of heat- and mass-transfer processes under microgravity. The distribution and size of dispersed phase are very essential for the analysis of heat and mass transfer, pressure drop and flow pattern in two-phase system. There is a great need to study how the bubble size and frequency can be controlled in microgravity.

Progress During FY 1996:

This is a new grant started on July 1, 1996. The PI just started designing a ground-based test setup to study the effect of thermocapillary flow on bubble generation. The PI is also constructing a test setup for microgravity isothermal experiments aboard the DC-9 aircraft of NASA/Lewis.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-191

RESPONSIBLE CENTER: LeRC

Instability of Velocity and Temperature Fields in the Vicinity of a Bubble on a Heated Surface

PRINCIPAL INVESTIGATOR: Dr. Mohammad Kassemi

Ohio Aerospace Institute

CO-INVESTIGATORS:

Rashidnia, N.

NYMA, Inc., NASA Lewis Research Center (LeRC)

Task Objective:

The objective of this combined experimental/numerical work is to investigate the fluid flow and temperature fields in the vicinity of a bubble attached to a heated solid surface. The goal of the research is to investigate the interaction between thermo-capillary and natural convective flows in the vicinity of the bubble in both low-g and 1-g environments and to identify numerically the parametric range for which unsteady periodic oscillations occurs on Earth.

Task Description:

The ground-based research activity includes the development of a numerical model, and experimental set-up, procedures, and diagnostic techniques needed for studying the time evolution of thermocapillary and natural convective flows in the vicinity of a gas bubble placed on a heated surface. The accuracy of the model is assessed by comparing numerical predictions to experimental measurements. Hand-in-hand numerical simulations and carefully controlled experiments are used to clarify the interaction between natural convection and thermocapillary convection and its effect on initiation of temperature and flow field oscillations. The verified numerical model is used to predict the steady state bubble shape, temperature field, and flow structure in the low-g environment. Various parametric simulations will be conducted to see if the oscillatory phenomenon is also present in the microgravity space environment and to delineate the origin and nature of the oscillations.

Task Significance:

The oscillatory thermo-capillary phenomenon is not only of fundamental importance in understanding the behavior of fluid flow in space but it also has practical significance in terrestrial applications. For example, in crystal growth, the oscillatory temperature and flow fields created by unavoidable bubbles next to the solid-liquid interface may seriously affect the quality of the emerging crystal and in nucleate boiling the presence of bubbles on the solid surface may increase the heat transfer rates considerably. The results of this investigation will enhance our understanding of the role of capillary forces in fluid management, boiling processes, and materials processing for both space and ground-based applications.

Progress During FY 1996:

Research in FY96 progressed along both numerical and experimental fronts. The test cell setup was modified to

1. Improve bubble size control.
2. Extend the flexibility of the experiments by providing different operational temperature ranges.
3. Increase the accuracy of temperature measurements to a resolution of .01 degrees.

The diagnostic techniques were also improved. The original Point Diffraction Interferometry (PDI) was replaced by Mach-Zehnder Interferometry (MZI) while at the same time efforts were devoted to adopt the Wollaston Prism Interferometry (WPI) technique. Work is proceeding on development of an Abel transformation computer code to extract temperature data from the interferometry results. Finally, the laser sheet flow visualization techniques was improved by using different particles. Experimental data was collected to capture both steady-state and oscillatory modes. The oscillatory modes recorded included symmetric, asymmetric, and nonperiodic flows.

As part of the theoretical/numerical study, the equations describing the temperature and fluid flow fields around the bubble were formulated and cast into dimensionless form using appropriate scaling parameters. A finite element numerical model was developed and used to simulate the temperature and flow fields around the bubble. Ground-Based steady state temperature and velocity fields predicted by the finite element model are in excellent qualitative agreement with the experimental results obtained in our laboratory. More rigorous quantitative

comparisons are near completion. Low gravity simulations were also performed and indicated that the flow field, temperature profile and bubble shape in the reduced gravity environment are significantly different from those obtained on earth. Recently, Wosniak and Wosniak (Exp. Fluids, 1996) reported the results of their low gravity experiment conducted aboard the TEXUS 33 sounding rocket. Our numerical predictions for bubble shape and temperature and flow fields are in excellent agreement with their experimental results. Based on these preliminary simulations and experimental results, the following conclusions can be made:

- Both experimental observation and numerical predictions indicate that the thermocapillary flow induced by bubbles on earth is greatly influenced and affected by its inevitable interactions with buoyancy-driven convection

- Both experimental observation and numerical predictions indicate that the low-g shape of the bubble, and the temperature and fluid flow fields are all drastically different from their terrestrial counterparts. More controlled low gravity experiments are needed to confirm these preliminary steady-state numerical predictions.

- Preliminary interferometric measurements in our laboratory demonstrate that the flow and temperature fields around the bubble can go through various oscillatory modes depending on the parametric space of the experiment. The nature and origin of these modes and their dependence on the interactions between natural and thermocapillary convection are as of yet not clearly known.

- Results and conclusions obtained during ground-based experiments with regard to oscillatory convection cannot in any way be extrapolated to determine the behavior of the thermocapillary flow in space

A transient finite element model was developed to study the time evolution of thermocapillary convection and temperature field around the bubble. Preliminary transient simulations indicate that when the bubble is subjected to the imposed axial temperature gradient, a strong thermocapillary flow is initiated. Eventually, a recirculating vortex develops close to the bubble and the hot plate. As the flow intensifies, the center of the vortex tends to move downwards. In 1-g the buoyancy force keeps the center of the vortex in the vicinity of the bubble. As the flow stabilizes the shear force exerted by it on the fluid below the bubble induces secondary and tertiary recirculating cells. Low-G simulations, however indicate that in the absence of the buoyancy force in low gravity, the thermocapillary vortex can grow and expand until it occupies the whole domain.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 12/94 EXPIRATION: 12/96

PROJECT IDENTIFICATION: 962-24-05-56

NASA CONTRACT NO.: NCC3-405

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Mercer, C.R., Rashidnia, N., and Creath, K., High data density measurement of quasi-steady-state flows. EXP. FLUIDS, 21, (1996).

Proceedings

Rashidnia, N., "Instabilities around a bubble due to combined Marangoni and Buoyancy Effects." Proceedings of the AIChE Symposium Series, published paper, vol. 92, no. 310, pp. 110-118, 1996.

Presentations

Kassemi, M. and Rashidnia, N., "Thermocapillary and natural convective flows generated by a bubble in 1-g and low-g environments." AIAA 34th Aerospace Sciences Meeting and Exhibit, Reno NV, AIAA 96-0734, January 1996.

Kassemi, M., Rashidnia, N., and Mercer, C., "Low-g and 1g velocity and temperature fields in the vicinity of a bubble on a heated surface." The Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, Ohio, June 1996.

Rashidnia, N., Kassemi, M., and Mercer, C., "Instabilities around a bubble due to combined Marangoni and buoyancy effects." ASME National Heat Transfer Conference, Houston, Texas, August 1996.

Stabilization of Thermocapillary Convection by Means of Nonplanar Flow Oscillations

PRINCIPAL INVESTIGATOR: Prof. Robert E. Kelly

University of California, Los Angeles

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

It has been demonstrated theoretically that small amplitude, nonplanar flow oscillations can stabilize Rayleigh-Benard convection. The first goal of this research is to discern if similar stabilization can be achieved for the thermocapillary (Marangoni) instability by the same means.

Task Description:

An asymptotic expansion based on Reynolds number will be used to perform stability analysis on both Rayleigh-Benard and Marangoni-Benard convection. A numerical approach using a Fourier representation in the horizontal directions and a spectral approach in the vertical direction will be used to obtain a coupled set of ordinary differential equations in time which can be solved by use of Floquet theory.

Task Significance:

If stabilization is possible, then the effects of finite amplitude oscillations will be determined in order to see how much stabilization is possible. And if significant stabilization is predicted, an experiment will be proposed at a later time.

Progress During FY 1996:

During the final year of this research project, emphasis was placed on understanding better the destabilizing effects of unsteady shear upon thermocapillary convection that can occur under microgravity conditions. This result is in contrast to our predictions for the earth-bound case, for which substantial stabilization seems to be possible. The destabilizing tendency was traced to an interfacial mode of instability that is created by the shear and that is primarily hydrodynamic in nature. It was discussed first for the case of an isothermal fluid layer by Yih in 1968, who found that a large wavelength mode of instability is possible. Before extending the analysis to the case of a heated layer of liquid, we decided to examine Yih's problem for finite wavelengths by use of a numerical method. We found a series of large wavelength modes (in a loop shape) in the relationship between critical Reynolds number and nondimensional frequency, β . However, we also found finite wavelength modes branching off those loops. These new modes are the most unstable ones for certain ranges of Reynolds number (Re) and nondimensional frequency, β . With these results established, we were able to return to the case of a heated layer in order to complete the analysis of thermocapillary convection, which is now being done under the new grant (NAG3-1819). The isothermal results were presented at the meeting of the Division of Fluid Dynamics of the American Physical Society in November, 1995, and a paper based on the results was submitted to the Journal of Fluid Mechanics (a revised version of the paper is currently under review).

Student supported:

C. H. Chen is a Ph.D. student in the MAE Department who began to receive support from the grant during the summer of 1995. He is investigating the effect of unsteady shear upon the subcritical development of Marangoni convection. This occurs in the form of hexagons for the case without shear. It is anticipated that the shear will inhibit the formation of hexagons and possibly eliminate the subcritical instability.

H. C. Hu was supported during the last part of 1995 and the first part of 1996 in order to complete an analysis of the effects of unsteady shear upon the onset of longitudinal vortices in a steady shear flow due to buoyancy or centrifugal effects. Although this analysis did not concern directly thermocapillary convection, it sets the stage for the analysis of this case when a steady flow component occurs in addition to the unsteady component. A paper based on this analysis has been submitted to Physics of Fluids.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 2/93 EXPIRATION: 4/96

PROJECT IDENTIFICATION: 962-24-05-56

NASA CONTRACT No.: NAG3-145

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Hu, H.C. and Kelly, R.E., Stabilization of longitudinal vortex instabilities by means of transverse flow oscillations. J. Phys. Fluids, (1996).

Or, A.C., Finite wavelength instability in a horizontal liquid layer on an oscillating plane. J. Fluid Mech., (1996).

Or, A.C., Finite wavelength instability in a horizontal liquid layer on an oscillating plane. J. Fluid Mechanics, (1996).

Or, A.C. and Kelly, R.E., Onset of Marangoni convection in a layer of fluid modulated by a weak nonplanar oscillatory shear. Ins. J. Heat Mass Transfer, vol. 38, pp 2269-2280 (October 1995).

Or, A.C. and Kelly R.E., Finite wavelength instability of a free surface due to an oscillatory shear. Bull. Am. Phys. Soc., vol. 40, p 1949 (October 1995).

Studies in Thermocapillary Convection of the Marangoni-Bénard Type

PRINCIPAL INVESTIGATOR: Prof. Robert E. Kelly

University of California, Los Angeles

CO-INVESTIGATORS:

Hu, A. C.

University of California, Los Angeles

Chen, C. H.

University of California, Los Angeles

Task Objective:

It has been demonstrated theoretically that small amplitude, nonplanar flow oscillations can stabilize Rayleigh-Benard convection. The first goal of this research is to discern if similar stabilization can be achieved for the thermocapillary (Marangoni) instability by the same means.

Task Description:

This investigation consists of two parts. The first part is a continuation of the investigation begun in NAG3-1456 of the effects of unsteady shear upon thermocapillary convection of the Marangoni-Benard type. The second part concerns the effect of imperfections in boundary conditions upon the onset of thermocapillary convection. Research on this latter topic will begin only in the Fall of 1996 and so it will not be discussed further here.

Task Significance:

If stabilization is possible, then the effects of finite amplitude oscillations will be determined in order to see how much stabilization is possible. And if significant stabilization is predicted, an experiment will be proposed at a later time.

Progress During FY 1996:

It has been reported previously that an interfacial mode of instability caused by the unsteady shear limits the amount of stabilization achievable on Earth concerning the onset of thermocapillary convection via a bifurcation. Nonetheless, the critical Marangoni number can be increased by a factor of ten by the shear. In microgravity conditions, the effect of the destabilization of the interfacial mode tends to become dominant and leads to destabilization of the layer for certain values of nondimensional frequency. Recent calculations done during preparations for the Third Microgravity Fluid Physics Conference have suggested that the destabilization does not occur for all frequencies and that stabilization can occur for certain frequencies. This discovery is being investigated currently and is considered to be important because it indicates that the phenomenon is more frequency sensitive in the microgravity case than previously thought. Once this aspect of the investigation has been resolved, a paper will be prepared for publication that reports the results of our numerical calculations for finite values of the oscillation Reynolds number.

An effort is being made this summer to extend the general analysis to the case of two fluid layers bounded above and below by walls. The results for this case can be compared more exactly to any future experimental results than the case for a free surface, which has been considered thus far.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-181

RESPONSIBLE CENTER: LeRC

Two-Phase Annular Flow in Helical Coil Flow Channels in a Reduced Gravity Environment

PRINCIPAL INVESTIGATOR: Prof. Edward G. Keshock

Cleveland State University

CO-INVESTIGATORS:

Lin, Chin S.

Analex Corporation

Task Objective:

One of the primary objectives of the study is to identify the conditions under which the transition to annular flow occurs for two-phase adiabatic air/water flow in helical coil flow channels, and to make detailed measurements of the characteristics of that flow under the low-gravity conditions experienced in DC-9 aircraft flight testing. A second principal objective is to obtain accurate measurements of two-phase pressure drop characteristics in such simulated microgravity conditions (aided considerably by the very large channel lengths attainable through the use of a helical coil geometry, containable in a rather compact test volume). A third general objective is to obtain a more fundamental understanding of two-phase flow behavior in helical coils, which, under earth gravity conditions, is considerably more complex than that in straight channel flows.

Task Description:

The adiabatic two-phase flow of air and water will be studied by observing and measuring the flow characteristics in helical coil flow channels. Tests will be conducted under earth-gravity and low-gravity conditions, in a laboratory test cell and DC-9 aircraft, respectively.

Video photographic observations of flow patterns, their transitions, and flow details will be made using a transparent test section. Also, a pressure-differential measurement technique will be employed in an attempt to develop a passive method for identifying flow patterns in non-transparent flow channels.

Measurements of pressure drop will be made using a series of stainless steel coiled test sections and compared with comparable flows in straight flow channels, under both earth gravity and simulated microgravity conditions. The objective of such a comparison will be to develop a relationship between straight- and curved- channel flows. Such a relationship will make it possible to compare pressure drop measurements made in the long, coiled flow channel with predictive models for both 1-g and microgravity conditions, which have been almost exclusively developed for straight-channel flows.

The observed slug-annular flow pattern transition boundary will be compared with those predicted by flow pattern maps appearing in the literature.

Additional flow characteristics that will be measured include film thickness, void fraction, bubble size, size distribution, and velocity.

Task Significance:

Due to the scarcity of data and models available for accurately predicting two-phase pressure drop under microgravity conditions, a more accurate model for predicting pressure drop is likely to be a result of these studies which reflects channel curvature and the influence of secondary flows upon two-phase flow characteristics.

Similarly, it is expected that the conditions under which the transition to annular flow occurs may be accurately identified, such that modifications to existing flow pattern maps, or development of a more generalized flow pattern map are likely results.

Finally, the detailed flow characteristics that will be observed and measured under simulated microgravity conditions will be those of much simpler flows, i.e., flows unencumbered of the complicating effects induced by the presence of a 1-g environment. Consequently, this simplicity appears to provide the possibility for obtaining a better fundamental understanding of helical coil two-phase flows.

Progress During FY 1996:

A test program has been formulated in the sense of identifying a number of test sections of different geometries that will achieve the above-described experimental objectives. The required test sections have been designed for compatibility with an existing NASA test rig utilized in conducting a variety of two-phase flow experiments in the DC-9 aircraft and are in the process of being fabricated.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/96 EXPIRATION: 7/99

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NAG3-192

RESPONSIBLE CENTER: LeRC

Microgravity Heat Transfer Mechanisms in the Nucleate Pool Boiling and Critical Heat Flux Regimes Using a Novel Array of Microscale Heaters

PRINCIPAL INVESTIGATOR: Prof. Jungho Kim

University of Denver

CO-INVESTIGATORS:

Moore, C.

University of Denver

Task Objective:

The objectives are to determine the relative contribution of the various heat transfer mechanisms to the overall heat flux in a sub-cooled, nucleate pool boiling in a microgravity environment, and to obtain quantitative data measuring local heat transfer coefficients at critical heat flux conditions.

Task Description:

A two-dimensional array of microscale heaters will be used for these tests to provide control and make measurements. These heaters will be kept at a constant temperature and their power input will be measured to control the heat flux. With the ability to measure and control temperatures and heat flux over very small areas, it should be possible to adequately quantify some of the behavior during nucleate pool boiling and critical heat flux during various stages of bubble growth and departure. Testing is limited to normal gravity tests.

Task Significance:

The development of such a microscale heater could significantly enhance the state-of-the-art in scientific instrumentation in the area of flow boiling and two-phase flow. Understanding the boiling phenomena has tremendous impact on electronic cooling and the nuclear, oil, and electric power industries.

Progress During FY 1996:

The research to date has focused on the design and construction of a 148 heater array, and the development of an improved feedback loop circuit. At this time, the heater array has been constructed, and preliminary data regarding the heater resistance, power dissipation capability, and frequency response have been obtained. These data show that the heaters have very linear resistance vs. temperature characteristics, are able to dissipate at least 600 W/cm² of energy, and have frequency responses of 15 kHz. In addition, the heater resistance was found to be very stable with time. One problem was encountered regarding thermal cross-talk between individual heaters in the array due to the large thermal conductivity of the silicon substrate. The array is currently being rebuilt using a quartz wafer as the substrate to eliminate this problem.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	3	BS Degrees:	1
MS Students:	0	MS Degrees:	0
PhD Students:	0	PhD Degrees:	0

TASK INITIATION: 5/94 EXPIRATION: 5/96

PROJECT IDENTIFICATION: 962-24-05-87

NASA CONTRACT No.: NAG3-160

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Kim, J., Ch'ng, C.P., and Kalkur, T.S., Design of an improved heater array to measure microscale wall heat transfer. NASA Conference Publication, 3338, pp. 165-170 (1996).

Proceedings

Kim, J. and Kalkur, T.S., "Development of a surface array of microscale heaters to measure wall heat transfer underneath single bubbles in nucleate pool boiling." Proceedings of the ASME Winter Annual Meeting, San Francisco, CA, November 1995.

Presentations

Kim, J., and Kalkur, T.S., "A surface mounted array of microscale heaters for use in nucleate boiling." presented at the 1995 National Heat Transfer Conference, Portland, OR, August 1995.

Investigation of Pool Boiling Heat Transfer Mechanisms in Microgravity using an Array of Surface Mounted Heat Flux Sensors

PRINCIPAL INVESTIGATOR: Prof. Jungho Kim

University of Denver

CO-INVESTIGATORS:

Kalkur, T. S.

University of Colorado, Colorado Springs

Task Objective:

The objectives are to as follows:

1) to determine the relative contributions of various heat transfer mechanisms to the overall heat flux in subcooled, pool boiling of a fluorinert on a flat plate in microgravity environments; and 2) to obtain quantitative data on the effects of microgravity on critical heat flux levels.

Task Description:

A novel heater surface consisting of a two-dimensional array of microscale heaters will be used to measure the heat transfer from a surface at many points underneath a bubble in conjunction with visual data. This heater array will enable the heat transfer to a surface during the bubble growth and departure process to be measured with very high temporal and spatial resolution. Normal gravity testing and ground-based reduced gravity testing, aboard the DC-9 facility, will be performed.

Task Significance:

The development of such a microscale heater could significantly enhance the state-of-the-art in scientific instrumentation in the area of flow boiling and two-phase flow. Understanding the boiling phenomena has tremendous impact on electronic cooling and the nuclear, oil, and electric power industries.

Progress During FY 1996:

This effort is based on a prior NRA award, NAG3-1609, "Microgravity Heat Transfer Mechanisms in the Nucleate Pool Boiling and Critical Heat Flux Regimes Using a Novel Array of Microscale Heaters," and was selected for award in the 1994 Fluids NRA, NRA-94-OSSA-05.

The research to date has focused on building a new heater array on a quartz substrate to eliminate the problem of substrate conduction, and the design of an improved feedback loop. The frequency response of an individual heater element was measured recently to be 15 kHz. Preliminary data obtained under the previous contract showed that the heaters have very linear resistance vs. temperature characteristics, and are able to dissipate at least 600 W/cm² of energy. In addition, the heater resistance was found to be very stable with time.

New masks for the heater array construction have been built, and a source to get silicon deposited on quartz has been identified. The new heater array will also have a small 3 micrometer square cavity at the center of the array to serve as a nucleation site. Improvements to the feedback loop include using a multiplier chip in place of the voltage controlled resistor, and an improved heater calibration capability.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 2
MS Students: 0
PhD Students: 0

TASK INITIATION: 6/96 **EXPIRATION:** 6/00**PROJECT IDENTIFICATION:** 962-24-00**NASA CONTRACT NO.:** NCC3-470**RESPONSIBLE CENTER:** LeRC

Molecular Dynamics of Fluid-Solid Systems

PRINCIPAL INVESTIGATOR: Prof. Joel Koplik

City College of New York

CO-INVESTIGATORS:

Banavar, J.R.

Pennsylvania State University

Task Objective:

The objective of this theoretical research is to examine the molecular behavior of fluids in confined geometries and near boundaries using molecular dynamics calculations and the statistical mechanics of classical fluids. It looks at time and spatial scales where continuum fluid mechanics provides no insight.

Examples investigated include (1) non-Newtonian fluid flows (2) phase separation of thin films of fluid mixtures (3) the breaking and coalescence of droplet interfaces driven by gravity or flows and (4) molecular scale studies of wetting and adhesion.

Task Description:

The numerical calculations are based on Molecular Dynamics, wherein one integrates the (classical) equations of motion for interacting molecules of various species, based on a prescribed interaction and specified thermodynamic operating conditions and mechanical forces. Within the framework of molecular dynamics, it is straightforward to impose a desired value of gravity or simulate the presence of g-jitter.

Task Significance:

We intend to carry out a number of calculations involving coexisting liquid, vapor and solid phases under flow conditions, with two common features. First, the systems will be studied at the molecular scale to obtain otherwise unavailable information. Second, the problems to be studied deal with fundamental issues in the physics of fluids and interfaces that are of relevance to the microgravity program.

Progress During FY 1996:

We have investigated two topics in non-Newtonian fluid flow, with publications now in preparation. The simulations are based on a microscopic model of the fluid, consisting of chain molecules made by bonding Lennard-Jones atoms together with nonlinear confining forces. In connection with forthcoming liquid bridge Shuttle experiments by McKinley, we have studied the extensional flow of a liquid cylinder. The results exhibit interesting differences compared to the (previously studied) Newtonian case. Secondly, to elucidate the nature of the stress singularity in non-Newtonian flows at contractions, we have computed the flow in a geometry containing a reentrant corner, and found evidence for enhanced (but still integrable) singular behavior.

Calculations of the fluid-fluid-solid contact line motion on various surfaces have provided direct evidence for surface roughness as the origin of hysteresis. The simulations considered the displacement of two immiscible fluids in a Wilhelmy-plate configuration, which allowed us to measure the force and angle as a function of velocity in a controlled manner. If the solid is smooth we find a single-valued variation of the microscopic contact angle with velocity, but a rough plate gives an open hysteresis loop. Initial results will be submitted for publication shortly, on-going studies address the details of the interfacial motion in the hysteretic case, and polymeric and heterogeneous fluid systems will be considered next.

We are taking a fresh look at the contact mechanics when a spherical particle is pressed on a solid surface. The continuum theories that describe this have several assumptions built in that are questionable or not generalizable to cases when the surface is rough or there is an intervening fluid layer. We are simultaneously studying the problem of the detachment of a solid particle from a surface due to a superimposed flow.

We are in the process of developing a portable massively parallel molecular dynamics code suitable for describing (one or more) fluids that are made up of simple molecules or chain molecules, have molecular walls and tunable interactions. Such a program would be vital for carrying out further studies of the non-Newtonian behavior of

flowing polymeric liquids, and additionally provide a computational structure for situations where very large scale simulations are called for.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 3

TASK INITIATION: 6/90 EXPIRATION: 12/95**PROJECT IDENTIFICATION: 962-24-05-43****NASA CONTRACT NO.: NAG3-119****RESPONSIBLE CENTER: LeRC**

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

d'Ortona, U., DeConinck, J., Koplik, J. and Banavar, J.R., Terraced spreading mechanisms for chain molecules. Phys. Rev., E 53, 562-569 (1996).

Dell'Aversana, P., Banavar, J.R. and Koplik, J., Suppression of coalescence by shear and temperature gradients. Phys. Fluids 8, 15-28 (1996).

Kebblinski, P., Kumar, S.K., Maritan, A., Koplik, J., and Banavar, J.R., Interfacial Roughening Induced by Phase Separation. Phys. Rev. Lett. 76, 1106-1109 (1996).

Koplik, J. and Banavar, J.R., Corner flow in the sliding plate problem. Phys. Fluids 7, 3118-3125 (1996).

Koplik, J. and Levine, H., Scattering of superfluid vortex rings. Phys. Rev. Lett. 76, 4745-4748 (1996).

Vergeles, M., Kebblinski, P., Koplik, J. and Banavar, J.R., Stokes drag and lubrication flows - a molecular dynamics study. Phys. Rev. E 53, 4852-4864 (1996).

Presentations

Koplik, J. "Fluid flow at the molecular scale." Yale University, Mechanical Engineering Dept., November 1995.

Koplik, J., "Molecular Dynamics of Fluid Flow." Ohio State University, April 1996.

Koplik, J., "Molecular dynamics of fluid flow." Yale University, November 1995.

Koplik, J., "Molecular dynamics of fluid flow." Hunter College, February 1996.

Koplik, J., "Molecular dynamics of fluid flow." Brown University, April 1996.

Molecular Dynamics of Fluid-Solid Systems

PRINCIPAL INVESTIGATOR: Prof. Joel Koplik

City College of New York

CO-INVESTIGATORS:

Banavar, J.R.

Pennsylvania State University

Task Objective:

The objective of this theoretical research is to examine the molecular behavior of fluids in confined geometries and near boundaries using molecular dynamics calculations and the statistical mechanics of classical fluids. It looks at time and spatial scales where continuum fluid mechanics provides no insight.

Examples investigated include (1) flows and spreading of non-Newtonian fluids, (2) the origins and dynamics of wetting hysteresis, (3) molecular scale studies of the adhesion of solid particles to surfaces, and (4) the physics of colloidal hard sphere systems.

Task Description:

The numerical calculations are based on Molecular Dynamics, wherein one integrates the (classical) equations of motion for interacting molecules of various species, based on a prescribed interaction and specified thermodynamic operating conditions and mechanical forces. Within the framework of molecular dynamics, it is straightforward to impose a desired value of gravity or simulate the presence of g-jitter.

Task Significance:

We intend to carry out a number of calculations involving coexisting liquid, vapor and solid phases under flow conditions, with two common features. First, the systems will be studied at the molecular scale to obtain otherwise unavailable information. Second, the problems to be studied deal with fundamental issues in the physics of fluids and interfaces that are of relevance to the microgravity program.

Progress During FY 1996:

We have embarked on a study of the physics of hard spheres that relate to the upcoming Shuttle experiments of Chaikin and Russell. We have developed a molecular dynamics program for hard spheres that we are in the process of parallelizing. We have run tests of small systems along with a Stokesian Dynamics code to assess the impact of the hydrodynamic modes on the transport properties of the system. We have checked our molecular dynamics code by comparing our results quantitatively with the earlier work in the field on small size systems. Our immediate goal is to study the frequency dependent viscosity as a function of the shear rate and the packing fraction. We will also study the nature of ordering as a function of the volume fraction, the dynamics of crystallization and non-Newtonian effects due to ordering of the hard spheres at high shear rate.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 3

TASK INITIATION: 5/96 **EXPIRATION:** 5/00**PROJECT IDENTIFICATION:** 962-24-00**NASA CONTRACT NO.:** NAG3-183**RESPONSIBLE CENTER:** LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Dell'Aversana, P., Koplik, J. and Banavar, J.R., Suppression of coalescence by shear and temperature gradients. *Phys. Fluids*, vol. 8, no. 15, (1996).

Presentations

Banavar, J.R., "Continuum Deductions from Molecular Hydrodynamics." CECAM Conference "The Microscopic Approach to Complexity by Molecular Simulations", Lyon, July 1996.

Banavar, J.R., "Continuum Deductions from Molecular Hydrodynamics." 6th International Conference on Discrete Models for Fluid Mechanics, Boston (Aug. 1996).

Koplik, J., "Molecular dynamics of fluid flow." Third NASA Fluids Conference, Cleveland (June 1996).

Koplik, J., "Molecular dynamics of fluid flow." Universite de Paris - Orsay, June 1996.

Thermocapillary Convection in Floating Zones under Simulated Reduced Gravity

PRINCIPAL INVESTIGATOR: Prof. Sindo Kou

University of Wisconsin, Madison

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The main objective of the research is to enable comparison between calculated and observed patterns of thermocapillary convection in floating zones, regardless of whether or not the zones are cylindrical in shape.

Ground-based flow visualization experiments will be conducted under simulated reduced-gravity conditions, i.e., where thermocapillary convection dominates over natural convection just as in microgravity. This will include silicone-oil zones and molten zones in NaNO_3 rods. Computer simulation of thermocapillary convection will be conducted and the calculated results will be compared with those observed in flow visualization.

Task Description:

A mathematical formulation will be used to quantitatively describe the optical distortions. This formulation allows the calculated flow patterns and solid/liquid interfaces to be converted into distorted ones so that they can be compared directly with those observed in flow visualization to verify the validity of computer simulation. Conversely, it can also be used to convert the observed flow patterns and solid/liquid interfaces into undistorted ones.

Task Significance:

Comparisons between calculated and observed patterns of thermocapillary convection in floating zones, though significant, have been rare (if performed at all), due to complications from optical distortions caused by the lens effect of the floating zones. With the numerical tool, thermocapillary flows in floating zone configurations can be more deeply understood. The capability of prediction can help the design of process active control, thus the quality of the material and medicine will be improved.

Progress During FY 1996:

1. High Pr materials: The work on silicone oil zones was published after revision of the original manuscript submitted for publication.
2. Low Pr materials: Extension from high to low Pr materials was initiated. First, search was made to find a low Pr material which satisfies the following criteria: 1. a high enough surface tension, γ , to sustain a small liquid bridge, 2. a significant $d\gamma/dT$ to develop thermocapillary flow, 3. well-documented physical properties. A low melting point material tin was selected. Second, search was made to find a rod material which satisfies the following criteria: 1. good wettability by molten tin, 2. chemical compatibility with molten tin, 3. higher melting point than tin. Iron was selected. Third, a Pyrex glass vacuum chamber was made to protect the molten metal from air, which causes the free surface to be covered with an oxide film to interfere with or even suppress thermocapillary convection.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 2

TASK INITIATION: 12/92 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-24-05-46

NASA CONTRACT NO.: NAG3-139

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Tao, Y., Xiong, B., and Kou, S., Thermocapillary velocity in a molten NaNO_3 zone. (1996).

Y. Tao, B. Xiong and S. Kou, Thermocapillary velocity field in a silicone oil zone. International Journal of Heat and Mass Transfer, (1996).

Thermocapillary Convection in Low Pr Materials under Simulated Reduced-Gravity Conditions

PRINCIPAL INVESTIGATOR: Prof. Sindo Kou

University of Wisconsin

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The main objective of the research is to enable comparison between calculated and observed patterns of thermocapillary convection in floating zones, regardless of whether or not the zones are cylindrical in shape.

Ground-based flow visualization experiments will be conducted under simulated reduced-gravity conditions, i.e., where thermocapillary convection dominates over natural convection just as in microgravity. This will include silicone-oil zones and molten zones in NaNO_3 rods. Computer simulation of thermocapillary convection will be conducted and the calculated results will be compared with those observed in flow visualization.

Task Description:

A mathematical formulation will be used to quantitatively describe the optical distortions. This formulation allows the calculated flow patterns and solid/liquid interfaces to be converted into distorted ones so that they can be compared directly with those observed in flow visualization to verify the validity of computer simulation. Conversely, it can also be used to convert the observed flow patterns and solid/liquid interfaces into undistorted ones.

Task Significance:

Comparisons between calculated and observed patterns of thermocapillary convection in floating zones, though significant, have been rare (if performed at all), due to complications from optical distortions caused by the lens effect of the floating zones. With the numerical tool, thermocapillary flows in floating zone configurations can be more deeply understood. The capability of prediction can help the design of process active control, thus the quality of the material and medicine will be improved.

Progress During FY 1996:

1. For the first time a liquid bridge was set up to study thermocapillary convection in a low Pr material. A liquid bridge of molten tin was set up between two iron rods of 4.5 mm diameter in a Pyrex vacuum chamber.
2. A stainless steel vacuum chamber was built, which allowed easier sample and thermocouple loading/unloading than the Pyrex vacuum chamber. Subsequent experiments were conducted in the stainless steel chamber.
3. Flow oscillation was detected, with a thermocouple, in a liquid bridge of a low Pr material for the first time. The temperature oscillation was recorded on a strip chart recorder, which was fast enough for the oscillation frequency and amplitude to be determined but not enough for the detailed characteristics of oscillation to be analyzed. A computer data acquisition and processing system will be put together in the second half of 1996 for the experiments.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 4/96 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-190

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Tao, Y. and Kou, S., "Thermocapillary convection in low Pr materials under simulated reduced gravity." Third International Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 13-15, 1996.

Electric Field Induced Interfacial Instabilities

PRINCIPAL INVESTIGATOR: Dr. Robert E. Kusner

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

Min, K.Y.

Wu, X.L.

Onuki, A.

NASA Lewis Research Center (LeRC)

University of Pittsburgh

Kyoto University, Japan

Task Objective:

The objective of this work is to study the stability of a non-polar binary critical mixture interface in the presence of a electric field. The onset of instabilities and the steady patterns formed will be characterized.

Task Description:

Four task elements make up this work. In all cases the sample cells have a capacitor-like construction.

1. Optical observation of the onset and spatial structure of surface oscillations as a function of thermophysical properties, electric field strength, and fluid depth.
2. Use surface laser light scattering of thermal capillary waves or mechanically drive capillary wave techniques to measure the capillary wave dispersion relationship as a function of thermophysical properties, electric field strength, and fluid depth.
3. Measure the nucleation onset cloud point line as a function of electric field and quench temperature using laser light scattering.
4. Optical observation of the interfacial structure of a near-critical two-phase binary mixture during 5 Second Drop Tower experiments. The electric field is to be turned on during the drop.

Task Significance:

The dynamics of two-fluid free interfaces remain an area open for fundamental experimental and theoretical investigation. This work examines experimentally a unique situation where surface tension is controllable and an electric field influences the dynamics. Two related fluid systems of practical interest are the ferrofluid-air interface in the presence of magnetic fields and an electrolyte-air interface with charged ions in the presence of an electric field.

Progress During FY 1996:

Dr. Min officially began work on the project May 15. Dr. Kusner began work on June 1. Using reflected laser light from a near-critical hexane/perfluorohexane mixture interface at $T_c - 1K$, Drs. Kusner and Min have observed the signature of an instability at a field of about 10kV/cm, approximately in agreement with theory of Onuki. However, the diffracted beam did not indicate the presence of a hexagonally ordered array of surface undulations.

Work with a thinner cell, in order to increase the applied electric field, produced images of an interfacial instability at an electric field in excess of 15kV/cm. The instability manifested itself in a 1mm thick cell as an array of disordered columns approximately 100 microns in diameter. The density of the columns increased drastically with increasing field and decreasing proximity to the critical point. These preliminary results were presented at the 3rd Microgravity Fluids Conference, June 13-15.

A thermostat has been built to control the temperature of the binary fluid cell to within 500 microK. Such temperature control is necessary to measure the cloud point of the binary fluid system. Lastly, the laser optics to measure the surface dynamics are being redesigned since preliminary attempts to measure the spectrum of surface riplons with a 5mW HeNe laser has failed.

Interim results can be found on the WWW at <http://sound1.lerc.nasa.gov>.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 0

PhD Students: .5

TASK INITIATION: 4/96 EXPIRATION: 4/99

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAS3-278

RESPONSIBLE CENTER: LeRC

Analysis of Phase Distribution Phenomena in Microgravity Environments

PRINCIPAL INVESTIGATOR: Prof. Richard T. Lahey

Rensselaer Polytechnic Institute

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to map the void distribution throughout the tube cross-sectional area in two-phase flows. The principal flow patterns to be studied are the bubbly and slug-flow regimes.

Task Description:

The research approach is to conduct normal gravity testing using equal density simulation experiments. Normal gravity experimental data, as well as available microgravity data, will be used to verify computational fluid dynamic models that are being developed. Two types of equal density simulations will be used: liquid with solid spheres, and a pair of immiscible liquids.

Task Significance:

The orientation of the phases with respect to each other and the tube wall affects the heat transfer characteristics and the work required to pump the two-phase mixture. Terrestrial applications include the nuclear, electric power and oil industries.

Progress During FY 1996:

Discrete phase distributions were obtained using simulated microgravity conditions by using equal-density, immiscible liquid experiments such as either n-butyl benzoate or silicon oil as the dispersed phase in water at 20°C. For the conditions investigated, peaking of the gas phase was not observed near the wall. A new two-fluid model was developed and predicts the behavior well. The results suggest that the discrete phase (vapor) will not tend to accumulate close to the wall (a potentially dangerous situation).

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 12/92 EXPIRATION: 11/95

PROJECT IDENTIFICATION: 962-24-05-72

NASA CONTRACT NO.: NAG3-140

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Singhal, M., Bonetto, F., Lahey, R., Phase distribution phenomena for simulated microgravity conditions: experimental work. NASA Conference Publication, 3338, pp. 133-140 (1996).

Presentations

Singhal, M., Bonetto, F., Lahey, R., "Phase distribution phenomena for simulated microgravity conditions: experimental work." NASA Contractor Report 198461, March 1996.

The Breakup and Coalescence of Gas Bubbles Driven by the Velocity Gradients of a Non-Uniform Flow

PRINCIPAL INVESTIGATOR: Dr. L. G. Leal

University of California, Santa Barbara

CO-INVESTIGATORS:

Trinh, E.H.

Jet Propulsion Lab, Pasadena, CA (JPL)

Task Objective:

The objective is to study the interaction and coalescence of neutrally buoyant drops using a four-roll mill.

Task Description:

Preliminary studies of interaction (and possible coalescence) of neutrally buoyant drops would be carried out.

Imaging and flow control systems of an existing flow cell would be modified to account for out of plane interactions.

Once experimental results are available, we plan to carry out BI (Boundary Integral) simulations, especially of systems that we believe to be characteristic of clean interfaces. These will corroborate the clean surface assumption prior to experimental investigation of additive effects. They will also assist in understanding the physics during the thin film phase when direct visualization is difficult.

Task Significance:

The deformation, breakup, and coalescence dynamics of drops and bubbles are of fundamental concern in many 1-g processes, and are of greater importance for 0-g applications.

In 0-g, the usual mechanisms of buoyancy-driven coalescence are lost. Although thermocapillary-driven coalescence may sometimes become important, in many cases it will be coalescence driven directly by velocity gradients of a flow that is the dominant mechanism.

The four-roll mill generates ideal flow fields to study these dynamics of neutrally buoyant particles or cluster of particles. This work will pave the way to microgravity studies on non-neutrally buoyant (e.g., bubbles), surfactants, and non-Newtonian systems. Some preliminary ground-based work is possible using acoustic centering systems to counteract the effects of gravity.

Such a 'flow facility', when operated in microgravity, will facilitate studies on non-neutrally buoyant systems in a variety of steady and time-dependent flows, and may be applicable to many systems beyond the coalescence studies of this project.

Progress During FY 1996:

This is a new grant starting in FY96.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 11

TASK INITIATION: 6/96 EXPIRATION: 6/98

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NAG3-189

RESPONSIBLE CENTER: LeRC

Oscillatory Cross-Flow Electrophoresis: Application to Production Scale Separations

PRINCIPAL INVESTIGATOR: Dr. David T. Leighton

University of Notre Dame

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The task objective primarily consists of an experimental verification of the expected performance of an oscillatory cross-flow binary separation device. This device is designed to use an oscillatory electric field across the narrow gap of a specially designed electrophoresis channel to cause species with different electrophoretic mobilities to have different time/location histories within the gap. This oscillatory motion is coupled with an oscillatory fluid cross-flow to achieve rapid separation of molecules based on their electrophoretic mobilities. The system acts as a semi-permeable barrier, actively transporting molecules with mobilities either greater or lower than some adjustable value across the cell, while rejecting all others. Because the throughput is largely governed by the amplitude of the oscillatory cross-flow, protein throughputs several orders of magnitude greater than those in conventional continuous free-flow electrophoresis devices are theoretically achievable.

Task Description:

Initially, the design for the oscillatory cross-flow binary separation device will be finalized and the device itself constructed. After construction of the device, its performance will be first tested using the protein Bovine Hemoglobin (BHb). As the amplitude of the electric field is changed, the protein will be selectively driven via the coupling of the electric field and fluid oscillations through the separation cell from one reservoir to another. Subsequently, quantitative measurements of the separation achieved by the device will be made using two proteins of differing mobility. These proteins will be chosen such that they can be analyzed using the UV absorption spectrometer available to the PI at the Department of Chemical Engineering of the University of Notre Dame. Concurrent with the experimental studies, we will also conduct simulations of the device to investigate the influence of more general electric fields and oscillatory cross-flows. It is hoped that these investigations will allow us to optimize the device and further improve the selectivity and throughput.

Task Significance:

Because the amplitude of the throughput is largely controlled by the amplitude of the fluid motion and only indirectly by the electrophoretic mobility, the throughput of this device is potentially several orders of magnitude greater than conventional free-flow electrophoresis devices. Experimental verification of the theoretical concepts underlying the proposed device are crucial, however. The research program is designed to 1) provide such verification and 2) to further optimize the system.

Progress During FY 1996:

To verify the analytical and numerical results of the BOCE technique, an experimental system including a binary separation cell, two reservoirs and an electrolyte bath was constructed. The cell allows continuous flow of solute in a buffer solution through a separation chamber 10.0 cm long, 3.0 cm wide, and 0.1 cm thick. The central separation chamber of the cell is machined from a plastic sheet that is divided into two halves to accommodate solute feed across the entire 3.0 cm channel width. Fluid is introduced at either end of the separation chamber by means of a stainless steel syringe connected to polypropylene fittings extending through the electrolyte bath and connecting to the reservoirs. The separation chamber is sandwiched between two regenerated cellulose membranes, supported by the electrode screens. Gas bubbles and Joule heat are removed by submerging the entire cell in an electrolyte bath open to atmosphere.

Preliminary experiments to verify that the interaction of a purely oscillatory shear flow with an oscillatory electric field can lead to the net convection of a single charged protein species were conducted using Bovine Hemoglobin (BHb) dissolved in a sodium acetate/acetic acid buffer of pH 4.5 and conductivity of approximately 325.0 $\mu\text{S}/\text{cm}$. These experiments demonstrated the dependence of the flux on the phase angle and wave form of the cross flow and the electric field. Experiments demonstrating the separation of two proteins using this device are expected to begin shortly.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 9/94 EXPIRATION: 3/97

PROJECT IDENTIFICATION: 962-24-08-16

NASA CONTRACT No.: NAG8-108

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Molloy, R.F., Gallagher, C.T., and Leighton, D.T. "Binary Oscillatory Crossflow Electrophoresis." Proceedings of the Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 13-15, 1996.

Low Dimensional Models for Thermocapillary Convective Flows in Crystal Growth Processes

PRINCIPAL INVESTIGATOR: Prof. A. Liakopoulos

Lehigh University

CO-INVESTIGATORS:

Blythe, P.A.

Lehigh University

Task Objective:

The objective of this work is to construct and validate low dimensional dynamical models of surface tension driven flows that are relevant to crystal growth processes. The models will be used to study process stability and the use of reduced-order models for control schemes.

Task Description:

A data base of 2-D, axisymmetric, and 3-D numerical solutions of the full nonlinear governing equations will be constructed using spectral element methods. These simulations are based on a variation formulation for unsteady viscous flow and an Arbitrary-Lagrangian-Eulerian description. The Karhunen-Loeve, K-L, procedure is used to determine spatial structures of the computed flow and thermal fields. Coupling of the K-L procedure with the method of weighted residuals for the full models will yield a low-dimensional representation of the flow system.

Task Significance:

Reduced-order models make feasible stability and bifurcation calculations for thermocapillary flows of practical interest. Furthermore, they can provide the basis for designing model predictive controllers for the suppression of instabilities that occur during crystal growth processes in a microgravity environment.

Progress During FY 1996:

In the period of October 1995 - October 1996 research has been directed toward the following tasks.

1. Construction of low-dimensional models.

We have successfully constructed and validated low-order models for transitional forced, free, and thermocapillary convective flows in cavities and channels and we have extended the methodology to problems with moving geometry and deformable meshes. Proper orthogonal decomposition has been applied to oscillatory thermocapillary convection data obtained by J. Xu and A. Zebib (J. Xu and A. Zebib, 1996 International Mechanical Engineering Congress). The spatial eigenfunctions were determined by applying the method of snapshots to numerical solutions of the full model. In all cases the most energetic modes contain the large scale features of the flow, while modes with lower fluctuation energy levels capture smaller scale features.

2. Collection of data from direct numerical simulations of thermocapillary flows in rectangular cavities.

Two configurations are under investigation: a) differentially heated open cavities of aspect ratio (width/height) $A = 1, 2, 4$, and b) open shallow cavities with spatially periodic temperature distribution imposed on the free surface. In case (b) the governing equations are solved in a computational domain consisting of a single module with periodic boundary conditions on the side boundaries. All simulations are time-accurate and they incorporate the flexibility of the free surface.

3. Analysis of interfacial instabilities.

We have focused our investigations on interfacial instabilities in two-layer Poiseuille flow. We have incorporated the effects of temperature and viscosity fluctuations in our analysis. The results indicate that temperature and viscosity perturbations have a pronounced effect on the interfacial mode of instability. This is in contrast to our findings on the stability of plane, single-layer, Poiseuille flow for liquids exhibiting exponential viscosity-temperature dependence.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0 BS Degrees: 0
 MS Students: 0 MS Degrees: 0
 PhD Students: 1 PhD Degrees: 1

TASK INITIATION: 6/94 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-24-05-88

NASA CONTRACT NO.: NAG3-163

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Gunes, H., Liakopoulos, A., and Sahan, R.A., Low-dimensional description of oscillatory thermal convection: The small Prandtl number limit. Theoretical and Computational Fluid Dynamics, (accepted 1996).

Liakopoulos, A. and Blythe, P.A., Low-dimensional dynamical models of transitional convective flows. Bull. Am. Phys. Soc., vol. 40, no. 12, p. 1955 (October 1995).

Journal interfacial instability. Int. Comm. in Heat and Mass Transfer, vol. 23, pp. 485-493 (November 4, 1996).

Pinarbasi, A. and Liakopoulos, A., The role of variable viscosity in the stability of channel flow. International Communications in Heat and Mass Transfer, vol. 22, no. 6, pp. 837-847 (October 1995).

Sahan, R.A., Liakopoulos, A., Gunes, H., Reduced dynamical models of nonisothermal grooved channel flow. Physics of Fluids, (accepted 1996).

Proceedings

Gunes, H., Sahan, R.A., and Liakopoulos, A., "Low-dimensional representation of transitional buoyancy-driven flow in a vertical channel with discrete heaters." Proceedings of the 1995 National Heat Transfer Conference, vol.1, A. Oregata and S.P. Mulay eds., ASME HTD-vol. 303, ASME press, pp.125-137, October 1995.

Presentations

Liakopoulos, A., "Low-dimensional dynamical models of thermal convection." Third Microgravity Fluid Physics Conference, Cleveland, OH, NASA CP 3338, pp 325-330, June 13-15, 1996.

Liakopoulos, A., "Low-dimensional models of transitional thermal convection." Cornell University, Ithaca, N.Y., October 22, 1996.

Liakopoulos, A., "Low-dimensional models of transitional flows." University of Maryland, College Park, MD., April 26, 1996.

Liakopoulos, A. and Blythe, P.A., "Low-dimensional dynamical models of transitional convective flows." APS Meeting, Irvine, CA, November 19-21, 1995.

Sahan, R.A., Gunes, H., and Liakopoulos, A., "Low-dimensional models for coupled momentum and energy transport problems." in Cooling and Thermal Design of Electronic Systems, C.H. Amon, ed., HTD-vol.319/EEP-vol.15, 1995 International Mechanical Engineering Congress, pp. 1-15, October 1995.

The Micromechanics of the Moving Contact Line

PRINCIPAL INVESTIGATOR: Prof. Seth Lichter

Northwestern University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

In the micro-gravity environment, the prime agent causing fluid motion is the force due to surface tension. This force arises due to the interaction between fluid molecules as well as between the fluid molecules and the molecules of the bounding solid. The goals of this research seek to relate these intermolecular forces to the magnitude of the surface tension force and to describe how the properties of the fluid are altered during motion.

Task Description:

Our research is focused on describing (i) the density and dipole moment distributions of a static fluid in the neighborhood of the contact line, and (ii) the variation of fluid viscosity due to contact line motion. Concurrent theoretical, numerical and experimental investigations are pursued.

Task Significance:

Since it is frequently desirable to know how, in a given geometry, fluid flow is altered by the properties of the solid substrate and the liquid, relating the intermolecular material properties to the macroscopic features is a prerequisite for predicting how best to select a solid and liquid for producing a desired fluid behavior. In addition, the results of this work could aid in the design of customized materials for a given application. Such capabilities are essential for the design of capillary controlled systems, particularly those encountered in fluids management systems aboard spacecraft, but also for myriad applications on Earth.

Progress During FY 1996:

In the first three months of our research we have focused on describing the density and dipole moment distributions of the fluid. In the first months of our research, as a trial problem, we computed an analytic expression for the density distribution for the liquid/vapor interface. We now turn to finding the density distribution in the more complicated geometry of the neighborhood of the contact line. We have also set up an experimental method designed to measure dipole orientation at the surface of a conductor. The density and dipole moment distributions are uniform throughout the fluid except within the molecularly thin layers between the liquid and the solid and between the liquid and the ambient gas. Though of very limited extent, it is the property variations within these thin layers which set the values of the contact angle and interface curvature.

Lastly, we have also begun to analyze the available published data on how contact angle depends on the speed of the contact line. For systems without a moving contact line, the material properties of the fluid do not depend on the velocity field. However, for flows possessing a moving contact line, fluid properties within the thin interfaces do depend on the motion. Preliminary analysis of the data indicates that the fluid viscosity in the neighborhood of the contact line may depend on flow speed. It is necessary to describe this variation in order to calculate the forces needed to generate fluid flow, or conversely, to predict the forces due to a given flow.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 3

TASK INITIATION: 6/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-189

RESPONSIBLE CENTER: LeRC

Absolute and Convective Instability and Splitting of a Liquid Jet at Microgravity

PRINCIPAL INVESTIGATOR: Prof. Sung P. Lin

Clarkson University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective is to establish a definitive role of the capillary, viscous, and inertial forces in the absence of gravity by using the fluid dynamics problem of the stability of a liquid jet as a vehicle. The objective will be achieved by reexamining known theories that can be verified completely only in microgravity. The experiments performed in the microgravity facility at NASA LeRC will enable the verification of the theory with experimental data. Of particular interest are the wavelengths and growth rates of instabilities in a convective Rayleigh-type jet. A wide range of Weber and Reynolds numbers will be studied, and any unexpected phenomena in microgravity that may require a new interpretation of dynamic capillary forces will be examined.

Task Description:

The results of the proposed work may provide benchmark knowledge in fluid dynamics when experimental results obtained in microgravity are compared with the known 0-g theories. As previously reported, the original approach was to design a rig to conduct one-g experiment during the first year (1993). It was subsequently decided to design and fabricate a rig able to conduct both low-g and one-g liquid jet experiments. Numerical modeling and preliminary rig designs were accomplished during the first two years. Ground-based low-g experiments took place during the third year in the LeRC 2.2 Second Drop Tower. Two drop campaigns were conducted during FY 96.

Briefly, a test liquid is stored in a compressed liquid cylinder and is driven by pressurized helium through a regulator. The test fluid passes through a series of sensors which measure temperature, pressure, and flow rates before reaching the nozzle through which the liquid jet emanates. The time evolution of the liquid jet is photographed with a high speed motion picture camera. The nozzle itself is disturbed at a controlled frequency so as to promote disturbances at particular values. Various fluids were tested at various flow rates and frequencies.

Task Significance:

The knowledge gained on the precise mechanism of various modes of jet breakup will allow one to improve and/or understand many existing important industrial processes. These processes include fire suppression, fuel spray formation (combustion of liquid fuels), film coatings, formation of various chemical sprays, and in the area of powder metallogy. Improvements of the efficiency of these types of processes may also bring about a drastic reduction in environmental pollution (e.g., removal of toxic material).

Progress During FY 1996:

The Clarkson drop rig has now 96 drops to its credit. The design, build-up, and any necessary modifications necessary for tower operations were completed shortly after the rig first arrived at LeRC on 22 June 1995. The first drop tests occurred on 28 June 1995. As previously reported, initial testing occurred during the mid-July and the mid-September 1995 time periods. The rig was then modified for operation at higher flow rates.

Testing subsequently resumed during October 1995. 34 drops occurred during this month. 24 of these tests occurred at Reynolds numbers that were on the order of ten times greater than previously accomplished (from about 15 to 160). A mixture of glycerin and water was used (59% glycerin) for these tests. Unfortunately the tests were of insufficient quality to provide quantitative data. The jets were plagued by nonlinearities introduced by the hardware. For the other 10 tests of October 1995, the fluid used was glycerin at low Reynolds numbers (on the order of 0.15). Data was successfully obtained on the transition between absolute and convective instabilities. During the April 1996 testing, 27 more tests were conducted. 8 of these tests were done with SAE 10W oil and 19 were done with 1000 cSt silicone oil. The tests were more successful; for which testing with the later fluid successfully identified the transition between absolute and convective instabilities.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 2
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/96 **EXPIRATION:** 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NAG3-189

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Lin, S.P. Regimes of jet breakup and breakup mechanisms. AIAA Progress Series, Recent Advances in Spray Combustion, (1996).

Lin, S.P. and Friedman, M. Non-equilibrium evaporation from a heated liquid layer. J. of Thermophysics and Heat Transfer, vol. 10, 497-503 (1996).

Absolute and Convective Instability of a Liquid Jet at Microgravity

PRINCIPAL INVESTIGATOR: Prof. Sung P. Lin

Clarkson University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective is to establish a definitive role of the capillary, viscous, and inertial forces in the absence of gravity by using the fluid dynamics problem of the stability of a liquid jet as a vehicle. The objective will be achieved by reexamining known theories that can be verified completely only in microgravity. The experiments performed in the microgravity facility at NASA LeRC will enable the verification of the theory with experimental data. Of particular interest are the wavelengths and growth rates of instabilities in a convective Rayleigh-type jet. A wide range of Weber and Reynolds numbers will be studied, and any unexpected phenomena in microgravity that may require a new interpretation of dynamic capillary forces will be examined.

Task Description:

The results of the proposed work may provide benchmark knowledge in fluid dynamics when experimental results obtained in microgravity are compared with the known 0-g theories. As previously reported, the original approach was to design a rig to conduct one-g experiment during the first year (1993). It was subsequently decided to design and fabricate a rig able to conduct both low-g and one-g liquid jet experiments. Numerical modeling and preliminary rig designs were accomplished during the first two years. Ground-based low-g experiments took place during the third year in the LeRC 2.2 Second Drop Tower. Two drop campaigns were conducted during FY 96.

Briefly, a test liquid is stored in a compressed liquid cylinder and is driven by pressurized helium through a regulator. The test fluid passes through a series of sensors which measure temperature, pressure, and flow rates before reaching the nozzle through which the liquid jet emanates. The time evolution of the liquid jet is photographed with a high speed motion picture camera. The nozzle itself is disturbed at a controlled frequency so as to promote disturbances at particular values. Various fluids were tested at various flow rates and frequencies.

Task Significance:

The knowledge gained on the precise mechanism of various modes of jet breakup will allow one to improve and/or understand many existing important industrial processes. These processes include fire suppression, fuel spray formation (combustion of liquid fuels), film coatings, formation of various chemical sprays, and in the area of powder metallogy. Improvements of the efficiency of these types of processes may also bring about a drastic reduction in environmental pollution (e.g., removal of toxic material).

Progress During FY 1996:

The Clarkson drop rig has now 96 drops to its credit. The design, build-up, and any necessary modifications necessary for tower operations were completed shortly after the rig first arrived at LeRC on 22 June 1995. The first drop tests occurred on 28 June 1995. As previously reported, initial testing occurred during the mid-July and the mid-September 1995 time periods. The rig was then modified for operation at higher flow rates.

Testing subsequently resumed during October 1995. 34 drops occurred during this month. 24 of these tests occurred at Reynolds numbers that were on the order of ten times greater than previously accomplished (from about 15 to 160). A mixture of glycerin and water was used (59% glycerin) for these tests. Unfortunately the tests were of insufficient quality to provide quantitative data. The jets were plagued by nonlinearities introduced by the hardware. For the other 10 tests of October 1995, the fluid used was glycerin at low Reynolds numbers (on the order of 0.15). Data was successfully obtained on the transition between absolute and convective instabilities. During the April 1996 testing, 27 more tests were conducted. 8 of these tests were done with SAE 10W oil and 19 were done with 1000 cSt silicone oil. The tests were more successful; for which testing with the later fluid successfully identified the transition between absolute and convective instabilities.

STUDENTS FUNDED UNDER RESEARCH:

BS Degrees: 1
 MS Degrees: 3
 PhD Degrees: 0

TASK INITIATION: 1/93 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-24-05-47

NASA CONTRACT No.: NAG3-140

RESPONSIBLE CENTER: LeRC

Magnetorheological Fluids in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Jing Liu

California State University, Long Beach

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This research investigates experimentally the influence of gravity in the formation of the equilibrium structure of magnetorheological fluids.

Task Description:

Magnetorheological (MR) fluids are colloidal suspensions whose rheological properties can be varied through the application of an external magnetic field. The key to this modification is the structure induced in the particles of the suspension. This work focuses on both equilibrium and nonequilibrium structures. We seek a better understanding of their dynamics, their effect on the rheological properties, and the influence of gravity to their formation. Our previous measurements are the basis for this effort. We will start our research by continuing our measurements on the dynamics in dilute samples and extending these to more concentrated samples. At the same time we begin our rheology measurements by comparing the properties of equilibrium structures to nonequilibrium structures. The basic experimental techniques for this work will be static laser light scattering, dynamic light scattering, optical microscopic imaging, and rheology.

Task Significance:

This research will help us to understand the basic physics of the structure formation in this so called "smart" material under the application of an external field. It will additionally provide guidelines for applications of MR fluids as technologically important materials. For example, this material can be used in automobiles as shock absorbers, clutch controls, robotic joint controls, etc., due to the viscosity change controlled by the field. In order to fully exploit the possibilities of MR fluids and to build more efficient devices, a better understanding is essential.

Progress During FY 1996:

Both static (SLS) and dynamic (DLS) light scattering measurements on very dilute ferrofluid emulsions were continued during FY96. When chains form due to an applied magnetic field very strong scattering can be observed in a band located in the plane perpendicular to the magnetic field lines. The shape of this intense band of scattered light depends on the length of the chains and on chain fluctuations. Our measured data of the band was well fitted by a distribution of Bessel functions - each corresponding to one single chain length. If, in a first approximation, we neglect the chain fluctuations, then the distribution of Bessel functions directly yields the chain length distribution.

In DLS we extended our previous measurements to higher field strengths. Cumulant analysis of the measured correlation functions yielded a short time self diffusion coefficient from which we calculated an apparent chain length N . Chain formation was found to be reversible at low field strength, i.e. for a given field strength an equilibrium chain length exists. For high magnetic field strengths, the chains grow indefinitely which means that in this case chain formation is irreversible. These results were supported by the SLS measurements mentioned above.

At high field strengths, extensive measurements of the short time diffusion coefficient during chain formation were performed for various volume fractions, two considerably different particle sizes, and at different scattering vectors. The apparent chain length was found to obey a power law $N \sim t^z$ with $z = 0.6$. This result is conform to the Smoluchowski theory of irreversible aggregation. Moreover, all our measurements at different volume fractions, different particle sizes, and different field strengths collapse into one single graph of apparent chain length vs. time when we use a rescaled time. The scaling factor reflects the fact that the Brownian motion of the aggregating particles - single particles and chains - is biased by the attractive dipole-dipole interaction induced by the magnetic field.

Chain formation is a diffusion limited and therefore very slow process in these very dilute ferrofluid emulsions. After about 2 hours, gravitational settling started to affect both SLS and DLS measurements and thus limited our study of the time dependence of chain formation. The structure formation caused by the magnetic field has also a drastic effect on the long time dynamics. The decay of the correlation function is clearly not single exponential. And, for certain scattering angles above a threshold field strength, we find pronounced oscillations in the long time tail of the correlation functions. Since these oscillations are only observed if chains longer than a certain threshold length exist in the sample, we believe that they are caused by chain fluctuations. Further measurements will clarify this point.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 2
PhD Students: 1

TASK INITIATION: 6/94 EXPIRATION: 12/96

PROJECT IDENTIFICATION: 962-24-05-90

NASA CONTRACT NO.: NAG3-163

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Felt, D. W., Hagenbuechle, M., Liu, J., and Richard, J., Experimental study of the rheological behavior of a magnetorheological fluid. *J. Rheology*, (1996).

Felt, D.W., Hagenbuechle, M., Richard, J., Liu, J. Rheology of a magnetorheological fluidand. *J. Intelligent Systems & Structures*, (September 1996).

Proceedings

Felt, D.W., Hagenbuechle, M., Richard, J., and Liu, J., "Rheology of a magnetorheological fluidand." Proceedings of the 5th Int. Conf. on Electrorheological Fluids, Magnetorheological Suspensions and Associated Technology, p. 738, University of Sheffield, UK, W. Bullough, World Science, 1996.

Liu, J. and Hagenbuechle, M., "Chain dynamics in a dilute magnetorheological fluid." Proceeding of the Third Microgravity Fluid Physics Conference, NASA Lewis Research Center, Cleveland, OH, June 13-15, 1996.

Liu, J., and Hagenbuechle, M., "Chain dynamics in a dilute magnetorheological fluid." Proceedings of NASA 3rd Microgravity Fluid Physics Conf., Cleveland, OH, June 13-15, 1996.

Presentations

Hagenbuechle, M., Sheaffer, P., and Liu, J., "Static dynamic light scattering of dilute magnetorheological emulsion." Gordon Conference on Macromolecular and Electrolyte Solutions, Ventura, CA, February 11-16, 1996.

Liu, J., "Recent development and research in electrorheological and magnetorheological fluids." Complex Fluid Workshop, Chinese Science Academy, September 23-27, 1996.

Liu, J., "Structure and dynamics of a ferrofluid emulsion in a magnetic field." Symposium on Complex Liquid American Physics Society, St. Louis, March 1996.

Liu, J., "Static and dynamic properties of chain formation in a dilute magnetorheological fluid." Symposium on Microgravity Science, Sixth International Space Conference of Pacific-Basin Societies, December 6-8, 1995.

Liu, J., "Field-induced phase transition and structures of ferrofluid emulsions." Seminar, Dept. of Chemistry, UCLA, November 17, 1995.

Liu, J. and Hagenbuechle, M., "Static light scattering study of chain formation in a dilute ferrofluid emulsion." American Physics Society March Meeting, St. Louis, March 1996.

Liu, J. and Hagenbuechle, M., "Experimental study of chain formation and chain dynamics in a dilute ferrofluid emulsion." American Physics Society March Meeting, St. Louis, March 1996.

Liu, J., Hagenbuechle, M., Sheaffer, P., and Zhu, Y., "Static and dynamic properties of chain formation in a dilute magnetorheological fluid." Advances in the Astronautical Sciences (6th ISOCPS), Vol. 91, 431, 1996.

Okumoto, S., Hagenbuechle, M., Liu, J., "Diffusing wave spectroscopy study of dipole dipole interacting Brownian particles." American Physics Society March Meeting, St. Louis, March 1996.

Rheology of Concentrated Emulsions

PRINCIPAL INVESTIGATOR: Prof. Michael Loewenberg

Yale University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this task is to develop numerical simulations that describe the flow of moderately concentrated emulsions in devices such as a Couette viscometer using a novel 3-D, boundary integral formulation. Couette viscometry experiments will be performed to test the predictions of numerical simulations. Since the effects of buoyancy will hamper a quantitative comparison between the results of the ground-based experiments and the computer simulations, a space-flight experiment will be designed for conclusive validation of the numerical results for a future investigation.

Task Description:

The proposed research focuses on flow of viscous, multiphase fluids under conditions where the dispersed-phase volume fraction is moderately high and drop deformation is significant. Numerical simulations will be developed to demonstrate this type of flows.

This formulation will rigorously describe the hydrodynamic and capillary interactions between deformable drops and between deformable drops and rigid, bounding walls. Couette viscometry experiments will be performed to test the predictions of numerical simulations. Since the effects of buoyancy will hamper a quantitative comparison between the results of the proposed ground-based experiments and the computer simulations, a space-flight experiment will be designed for conclusive validation of the numerical results.

Task Significance:

Emulsions are viscous, multiphase fluids that arise in a wide range of industrial applications. The results of this study will enhance our understanding for applications in advanced materials processing, environmental protection, enhanced oil recovery, food processing, and pharmaceutical manufacturing. It can provide attractive mechanical properties of incompatible polymer blends which could enhance the process of recycling plastics.

Progress During FY 1996:

Self-diffusion coefficients that describe cross-flow migration of nonBrownian drops in a dilute sheared emulsion were obtained by trajectory calculations. A boundary integral formulation was used to describe pairwise interactions between deformable drops; interactions between undeformed drops were described with mobility functions for spherical drops. The results indicate that drops have large anisotropic self-diffusivities which depend strongly on the drop viscosity and modestly on the shear-rate. Pairwise interactions between drops in shear-flow do not appreciably promote drop breakup.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-193

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Loewenberg, M. and Hinch, E.J. "Self-diffusion of drops in a dilute sheared emulsion." Third Microgravity Fluid Physics Conference, NASA Conference Publication 3338, pp. 579-584, 1996.

Investigation of Thermal Stress Convection in Nonisothermal Gases under Microgravity Conditions

PRINCIPAL INVESTIGATOR: Dr. Daniel W. Mackowski

Auburn University

CO-INVESTIGATORS:

Knight, R.W.

Auburn University

Task Objective:

The objective of this research is to theoretically study the phenomenon of thermal stress convection in a gas under microgravity conditions. Thermal stress is a phenomenon in which temperature gradients in the gas directly impart a stress to it and thereby lead to motion of the gas.

Task Description:

While Navier-Stokes equations provide a highly accurate description of the behavior of a fluid in the continuum limit and relates the stresses in a fluid to pressure gradients, velocity gradients and body forces, kinetic theory predicts that gradients of additional quantities can be related to fluid stresses. Specifically, temperature gradients in a gas cause thermal stresses. These additional stresses have been described by the Burnett contributions to the fluid stress tensor. However, they are not well understood and there still exist unanswered questions regarding the validity of the Burnett terms. Nevertheless in this research the Burnett equations will be incorporated into the momentum equations and numerically analyzed to predict the thermal stress convection in a gas under microgravity conditions. The absence of gravity unmasks these flows and renders them to be easily observed experimentally. This research will provide a preliminary design for a space-based experiment to observe thermal stress convection.

Task Significance:

The nature of this research is to unravel a poorly understood phenomenon that is masked by earth's gravity in terrestrial experiments. It is also believed to be of some importance in a particular method of crystal growth called the PVT (physical vapor transport) technique.

Progress During FY 1996:

This research has been initiated in June 1996. The task for the first year include modification to an existing numerical code for PVT modeling and calculation of thermal stress and thermal creep convection in a gas in a container with non-uniform surface temperatures.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/96 EXPIRATION: 5/98

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-188

RESPONSIBLE CENTER: LeRC

The Dissolution of an Interface Between Miscible Liquids

PRINCIPAL INVESTIGATOR: Prof. James V. Maher

University of Pittsburgh

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective is to measure the strength and time rate of disappearance of the dynamic interfacial tension of a binary mixture as it transitions from immiscible to miscible as a function of the density difference between the two pure liquids. The results are expected to resolve the ambiguous results from previous experiments and models. This is an Earth-based experimental activity.

Task Description:

The investigator will employ near-critical concentration binary mixtures made of liquids with varying density differences. A temperature change of the mixtures, causing a phase transition from immiscible to miscible, will produce an interface that gradually vanishes.

Surface Light Scattering (SLS) and specular reflected laser beam tracking of Mechanically Driven Capillary Waves (MDCW) will be used to measure the vanishing interface's surface tension with time. The investigator expects to establish which of these two techniques is most suitable.

The use of several liquid pairs for the mixtures will examine what dissolving interface properties are material specific and which are universal.

Convection will be a troublesome side-effect for this work. Methods of controlling it will be refined to avoid confusion in the data. The possible need of a low-gravity experiment hinges on convection.

Task Significance:

Multi-phase to one-phase transitions in commercial materials processing are common. The rate of mixing during such a phase transition often greatly influences the quality of the resultant mixture and the cost of getting an acceptable product. This work seeks to improve the understanding of the interplay of buoyant forces with diffusion and mechanical stresses at the interface as a subset of the factors influencing the rate of mixing.

Progress During FY 1996:

This grant began in late May 1996. A post-Doc has been hired and began work September 1. A graduate student began work on the first day of June. We have reassembled a surface light scattering apparatus and are now in the process of testing it out. Surface light scattering is sufficiently tricky that one expects a significant calibration stage, and that stage will go on during the next quarter.

In parallel with calibrating the apparatus, we have been making samples. Before we begin to make the expensive density matched samples, we need to learn to make reliable samples with minimal dust on the interface and acceptably small curvature. Large curvature due to wetting at the walls requires large containers to avoid curvature at the surface scattering zone. But we also wish to avoid a container so large that the time to reach thermal equilibrium becomes prohibitively long. We have now succeeded in making samples with a remarkably small amount of dust. Unfortunately, the cyclohexane-methanol mixture is a complete wetting mixture, and so it has significant curvature if there is a sidewall within a centimeter of the point of laser incidence. We are currently measuring light scattering to determine whether or not we can live with such a large curvature. I expect to make high quality measurements of the capillary wave dispersion relation for the cyclohexane-methanol system at equilibrium and to measure the analogous light scattering signals from the perturbed liquid-liquid interface. It will be from the differences of the perturbed interface from the equilibrium that we will learn whether or not we are ready to interpret data for systems which differ only in their density match.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 0

PhD Students: 1

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NAG3-183

RESPONSIBLE CENTER: LeRC

Controlling the Mobility of a Fluid Particle in Space by Using Remobilizing Surfactants

PRINCIPAL INVESTIGATOR: Prof. Charles Maldarelli

City University of New York

CO-INVESTIGATORS:

Papageorgiou, D.

New Jersey Institute of Technology

Task Objective:

This research program studies theoretically and experimentally how to use surfactants to control the mobility of the fluid interface of bubbles or drops moving through a continuous liquid phase. The interfacial mobility determines the drag exerted on the fluid particle as it is driven through the continuous phase. By controlling this mobility, the steady translational velocity of the drop can be manipulated independent of the force causing the particle to move, and this control may prove useful in material processing under microgravity which requires the management of thermocapillary driven bubbles and drops.

Task Description:

Surfactant affects the interfacial mobility by creating surface tension gradients which resist the interfacial flow: Surfactant molecules dissolved in either the continuous or drop phase kinetically adsorb from the bulk sublayer adjoining the interface onto the surface. Once adsorbed, the surfactant is convected by the surface flow to the trailing pole of the particle. Accumulation at the back end causes kinetic desorption into the bulk sublayer; this increases the sublayer concentration causing a diffusive flux of surfactant out into the bulk. At the front end, the kinetic adsorption depletes the sublayer, and forces a diffusive flux of surfactant from the bulk to the sublayer. At a steady state, diffusive, kinetic and convective fluxes balance, and a concentration gradient develops on the surface with the trailing pole larger than the leading pole. Since surfactant reduces the interfacial tension in proportion to its surface concentration, the leading pole is at a higher tension than the trailing pole. The leading pole tugs at the trailing pole, and this tangential action opposes the surface flow and hinders the interfacial mobility.

To use this retardation mechanism to manipulate the interfacial mobility, the kinetic and diffusive fluxes which maintain the concentration difference across the fluid particle must be controlled. Diffusive fluxes can be controlled by using bulk concentrations large enough to form surfactant aggregates; these aggregates act as sources of surfactant monomer thereby reducing the diffusion gradients and increasing the interfacial mobility. Kinetic fluxes are controlled by the kinetic exchange coefficient, which is determined by the surfactant structure. The overall goal is to investigate both of these mechanisms.

Task Significance:

The results can be used to control thermocapillary driven bubble motion, e.g., in a glass melt, and in the miscibility gap solidification of two phase composites. In each of these examples there is a need for controlling the thermocapillary migration velocity; in the movement of gas bubbles in a melt, it is desired to have as large a migration as possible. In the case of miscibility gap solidification, the object is to reduce the migration velocity as much as possible, so that phase separation does not occur.

Progress During FY 1996:

During this reporting period, the following have been accomplished:

THEORETICAL

1. A new model has been developed to describe the kinetic rate of exchange of surfactant molecules between a liquid/gas surface and the adjoining liquid sublayer. This model uses the Arrhenius rate law framework to formulate the rates of adsorption and desorption. In this framework, exchange rates are proportional to kinetic coefficients multiplied by Boltzmann factors; thus the adsorption and desorption rates are equal, respectively, to $\beta[\exp(-E_A/RT)]$ and $\alpha\Gamma[\exp(-E_D/RT)]$, where G is the surface concentration, E_A (E_D) is the activation energy for adsorption (desorption) and β (α) is the adsorption (desorption) rate constant. The adsorption activation energy is computed as the work done against the surface pressure to create a space equal to the area per molecule (at the existing surface density). The activation energy for desorption is divided into an attractive contribution which accounts for the van der Waals attraction between chains, and a repulsive contribution due to hydration forces between the polar head groups of the surfactant molecules.

The kinetic model was first used to develop a theoretical equation of state relating the surface tension to the surface concentration. The model constants in the equation of state (the kinetic ratio a/b and the activation energy parameters) were obtained by measuring the tension as a function of the surface concentration using the pendant bubble technique (see EXPERIMENTAL, below). The kinetic constants were established by using the kinetic model to simulate dynamic tension experiments using the pendant bubble technique (see EXPERIMENTAL, below). The new model provides improved agreement with both equation of state and dynamic tension measurements when compared to other models which do not formulate in a realistic way the activation energies, and allows for a more realistic accounting for the effect of surfactant adsorption on bubble motion.

2. During the first year, a preliminary hydrodynamic model was developed to describe the decrease in the translational velocity of a bubble moving in a continuous Newtonian liquid phase due to the Marangoni stresses originating from the adsorption of surfactant on the bubble surface. (As described above in the TASK OBJECTIVE AND DESCRIPTION.) This model was for creeping flow and buoyantly driven motion, and included bulk diffusive and kinetic transport. The model demonstrated that as the bulk concentration increases for surfactants with sufficiently large kinetic rates, diffusion outpaces interfacial convection, the surface concentration becomes uniform and the translational velocity increases. Thus the bubble velocity can be manipulated by changing the bulk concentration. (Only concentrations below the formation of aggregates were considered.) During this second year, the model was reformulated to include more realistic features: (i) thermocapillarity as the driving force for the bubble motion, and (ii) inertial effects (order one Reynolds number). Simulations again indicated that the interface can be remobilized at high bulk concentrations. In addition, at low concentrations where bulk diffusion is slow, and the surfactant collects in a stagnant cap at the back, the inclusion of initial effects can lead to the formation of a wake due to the zero interfacial velocity at the trailing pole.

EXPERIMENTAL

1. The pendant bubble technique was used to measure the equation of state. A pendant bubble is formed at the tip of a needle immersed in a (aqueous) surfactant solution with a given concentration, and an equilibrium monolayer is allowed to form on the pendant bubble surface. From a digitized video image of a silhouette of the bubble shape, the interface locus can be obtained and numerically compared to the Young-Laplace equation to measure the surface tension. The bubble area is then rapidly contracted and expanded, so that the amount of surfactant on the surface is conserved (negligible transfer to the bulk). The tension is measured as a function of the interface area or surface concentration by sequential capture of the interface shape to establish the equation of state.

Equations of state for homologous series of polyethoxylated surfactants were obtained by the pendant bubble technique. Two series were studied, one in which the polar group is varied and one in which the hydrophobe chain length is changed. The new equation of state is fitted to the measurements to obtain the dependence of the constants in the state equations (activation energy parameters and equilibrium kinetic ratio a/b) on the chain length and size of the polar group.

2. Values for the individual kinetic constants α and β were established by dynamic tension measurements using the pendant bubble technique. A bubble is either rapidly formed in a surfactant solution, and the tension reduction as surfactant adsorbs onto the initially clean interface is measured, or a bubble with an equilibrium monolayer is compressed and the increase in tension as surfactant desorbs is measured. A model of the surfactant mass transfer during the clean interface adsorption and re-equilibration was developed which includes bulk diffusion and the kinetic exchange at the surface as described by the new rate law. Model simulations provided the tension as a function of time, and when compared to the measurements, established the kinetic constants and the diffusion coefficient. The kinetic constants were obtained for a single homologous series of polyethoxylated surfactants in which the hydrophobe chain length was varied.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/94 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-24-05-90

NASA CONTRACT No.: NAG-1618

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Huang, W. and Maldarelli, C., The effect of surfactant on the motion of bubbles and drops. CISM Lecture Notes, (1996).

Pan, R., Green, J. and Maldarelli, C., Measurement of kinetic rate constants for a homologous series of polyethoxylated surfactants. Langmuir, (1996).

Pan, R., Green, J., Pollard, M. and Maldarelli, C., New kinetic and state equations for the adsorption of surfactant on an air/water interface, and measurements of state equation parameters for a homologous series of polyethoxylated surfactants. J. Colloid and Interface Science, (1996).

Stabilization and Low Frequency Oscillations of Capillary Bridges with Modulated Acoustic Radiation Pressure

PRINCIPAL INVESTIGATOR: Prof. Philip L. Marston

Washington State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objectives of this investigation are to: (1) investigate the response of liquid capillary bridges to acoustic radiation pressure excitation, and (2) acoustically suppress capillary breakup of long liquid bridges.

Task Description:

Liquid bridges surrounded by another liquid are studied in a modified Plateau tank apparatus. The liquid bridge is usually a silicone-oil/ tetrabromoethane mixture surrounded by water. The bridge length and location are adjusted to investigate the mode coupling of the radiation pressure of the surrounding ultrasonic field. The ultrasonic field has been mapped with a hydrophone. For dynamic studies, the spatial and temporal modulation of the radiation pressure is used to selectively excite mode resonances. After deactivating the transducers, mode frequency and rate of the free decay has been monitored optically. Static bridge shapes are measured with CCD cameras attached to digitizers and a personal computer. Conditions are being investigated experimentally and/or theoretically for acoustic stabilization of bridges surrounded by air as well as water.

Task Significance:

The proposed research furthers the understanding of the dynamics of capillary bridges which can lead to improved control of float-zone crystal growth processes. The research may also lead to an increase in dynamic gravity tolerance levels for liquid bridge related phenomena on the Shuttle.

Progress During FY 1996:

The primary effort in this recently expired grant was to exploit the acoustic radiation pressure coupling with the shape of a liquid bridge (demonstrated in our recent publication in Physics of Fluids) for the purpose of stabilization of an extended liquid bridge against break up. Cylindrical oil bridges were deployed between two posts in the water bath of a Plateau tank. In the absence of any applied stabilization, the bridge would naturally break when the slenderness ratio S of length to diameter was close to the Rayleigh-Plateau limit of 3.1416. By using an ultrasonic field to actively control the shape of the bridge, stable cylindrical bridges having S as large as 3.6 were achieved during the tenure of this grant. The instantaneous shape of the bridge was optically sensed and the parameters of the ultrasonic wave field were electronically controlled so as to quench the growth of the naturally unstable mode. The method of controlling the shape involves the redistribution of the acoustic radiation stresses applied to the surface of the liquid bridge. The experiment is summarized in the Third Microgravity Fluid Physics Conference Proceedings, pp. 475-480.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 6/94 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-24-05-91

NASA CONTRACT No.: NAG3-162

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Marr-Lyon, M.J., Thiessen, D.B., Marston, P.L., Active acoustic stabilization of capillary bridges significantly beyond the Rayleigh limit: experimental confirmation. Journal of the Acoustical Society of America, 99, 2540 (1996).

Marston, P.L., Capillary bridge stability in an acoustic standing wave: linearized analysis of passive stabilization with radiation pressure. Bulletin of the American Physical Society, 40, 1923 (October 1995).

Morse, S.F., Thiessen, D.B., and Marston, P.L. Capillary bridge modes driven with modulated ultrasonic radiation pressure. *Physics of Fluids*, 8, 3-5 (1996).

Thiessen, D.B., Morse, S.F., Marr-Lyon, M.J., Marston, P.L., Capillary bridge modes driven with modulated acoustic radiation pressure. *Bulletin of the American Physical Society*, 40, 1923 (October 1995).

Presentations

Marston, P.L., Marr-Lyon, M.J., Morse, S.F., and Thiessen, D.B., "Stabilization and low-frequency oscillation of capillary bridges with modulated acoustic radiation pressure." Third Microgravity Fluid Physics NASA LeRC Conference, June 13-15, 1996.

Passive or Active Radiation Stress Stabilization of (and Coupling to) Liquid Bridges and Bridge Networks

PRINCIPAL INVESTIGATOR: Prof. Philip L. Marston

Washington State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The primary objective is to acoustically stabilize liquid bridges against break-up from the Rayleigh-Plateau instability or from the response to g-jitter. A secondary objective is to explore other responses of bridges to radiation stresses and to investigate the stability and modes of networks of liquid bridges.

Task Description:

Acoustic stabilization of liquid bridges is investigated with appropriately designed ultrasonic fields. In one approach the spatial distribution of the acoustic radiation pressure on the bridge is actively adjusted so as to counteract the growth of the most unstable mode. This is achieved by optically sensing the shape of the bridge and electronic control of the drive to the ultrasonic transducers. Another approach involves selection of the acoustic field such that a local variation in the bridge radius should produce a compensating change in the local acoustic radiation pressure. The bridges for investigation include liquids surrounded by an immiscible host liquid and bridges in air. While the primary emphasis is on bridges deployed between two fixed posts, a variation of the deployment uses three or more posts and produces a bridge network.

Task Significance:

The research should give improved capabilities to manage fluids in low-gravity by achieving stabilization beyond the Rayleigh-Plateau limit. This may have application to float-zone crystal growth processes or to the containerless mixing of liquid species.

Progress During FY 1996:

Since the beginning of the grant in July 1996, the emphasis has been on improving the active acoustic stabilization mechanism originally demonstrated with support from the now expired NASA grant, "Stabilization and Low-Frequency Oscillation of Capillary Bridges with Modulated Acoustic Radiation Pressure." The current experiments stabilize a liquid bridge of oil in a Plateau tank water bath. Some of the improvements implemented include the following items: (i) the optical sensors were redesigned to avoid signal interference from room lights. Consequently it is now possible to acoustically stabilize a bridge with normal levels of background lighting. (ii) The acoustic stabilization field was modified to improve the ability to control the shape of the bridge. Cylindrical bridges have now been stabilized by this method with the slenderness ratio of length to diameter being as large as 3.8 in comparison to the natural Rayleigh-Plateau stability limit of 3.1416. The technologies required to apply the method for the stabilization of liquid bridges surrounded by a gas are also being studied.

The stability of the simplest form of bridge deployed from three posts is also under investigation for an oil bridge in a Plateau tank.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 7/96 **EXPIRATION:** 7/00**PROJECT IDENTIFICATION:** 962-24-00**NASA CONTRACT NO.:** NAG3-191**RESPONSIBLE CENTER:** LeRC

Study of Disturbances in Fluid-Fluid Flows in Open and Closed Systems

PRINCIPAL INVESTIGATOR: Prof. Mark J. McCready

University of Notre Dame

CO-INVESTIGATORS:

Chang, H.-C.

University of Notre Dame

Leighton, D.

University of Notre Dame

Task Objective:

The objective of this effort is to examine the different instabilities that can affect a liquid film during gas-liquid flow.

Task Description:

A generalized approach is being undertaken for gas-liquid flow in an open channel with finite length, with or without gravitational stabilization, as well as for the analytically simpler case of liquid-liquid rotating flows. Either gas-liquid low-gravity testing or comparison with existing low gravity data is planned.

Task Significance:

The presence of waves can enhance the heat transfer between phases but increase the energy required to pump the phases through a pipe network. Terrestrial applications include the nuclear, electric power and oil industries.

Progress During FY 1996:

In Sangalli et al. (1995), the first sufficiently controlled experiments were completed that could confirm the accuracy of weakly-nonlinear predictions of the supercritical nature of the instability and the saturation value of the amplitude. Kuru et al. (1996) presented experiments showing different generic mechanisms that lead to formation of transverse disturbances in gas-liquid flows. Gallagher et al. (1996) describe situations where, surprisingly (since experiments in all other systems suggest otherwise), short wavelength waves saturate at small amplitude even though a spectrum of much longer wavelength waves is unstable.

Kuru et al. (1995) described the utility of exact differential theories for predicting stability of two-layer systems and pointed out the serious limitations of the commonly-used "one-dimensional" models. Sangalli et al. (1996) described a new weakly-nonlinear theory, verified by experiments in a gas-liquid system, that three different physical mechanisms play a role in stabilizing linearly unstable interfacial waves and that dramatically different behavior occurs close to resonance where different wave modes travel at the same speed.

The overall significance of this work is that because several aspects of weakly - nonlinear theories for interfacial systems have been verified, many new problems can be attacked by this approach and be expected to be correct. The unexpected observation of stable short waves in the presence of unstable long waves means that more robust theories are needed. Kuru's (1996) transverse wave results should spur new efforts at theoretically solving this long standing problem. Kuru et al. (1995) and Uphold & McCready (1995) provide evidence that standard methods for predicting flow regimes in two-phase flows are not consistent with rigorous stability theory and this could be fundamentally flawed.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	0
MS Students:	1	MS Degrees:	1
PhD Students:	4	PhD Degrees:	2

TASK INITIATION: 12/92 **EXPIRATION:** 11/95**PROJECT IDENTIFICATION:** 962-24-05-55**NASA CONTRACT NO.:** NAG3-139**RESPONSIBLE CENTER:** LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Chang, H.-C., Demekhin, E.A., Kalaidin, E., and Ye, Y., Scalings of Spatio-temporal Dynamics on a falling film. *Physica Scripta*, (accepted 1996).

Chang, H-C., Demekhin, E.A., Kalaidin, E., and Ye, Y., Coarsening dynamics of falling film solitary waves. *Phys Rev E*, (accepted 1996).

Gallagher, C.T., McCready, M.J., and Leighton, D.T., Experimental investigation of a two-layer shearing instability in a cylindrical Couette cell. *Phys. Fluids*, (accepted 1996).

Kuru, W.C., Sangalli, M., Uphold, D.D., and McCready, M.J., Linear stability of stratified channel flow. *Int. J. Mult. Flow*, 21, pp 733-753 (October 1995).

McCready, M.J., and Chang, H.-C., Formation of large disturbances on sheared and falling liquid films. *Chem. Eng. Comm.*, 141-142, pp 347-358 (1996).

Sangalli, M., Gallagher, C.T., Leighton, D.T., Chang, H.-C. and McCready, M.J., Finite amplitude wave evolution at the interface between two viscous fluids. *Phys. Rev. Let.*, 75, pp 77-80 (October 1995).

Proceedings

Chang, H-C., Demekhin, E.A., and Kalaidin, E., "Scalings, self-similarity and statistics of interfacial turbulence on a falling film." SIAM conference proceedings, accepted 1996.

Kuru, W.C., Sangalli, M., and McCready, M.J., "Transition to Three-dimensional Waves in Cocurrent Gas-liquid Flows." SIAM conference proceedings, accepted 1996.

Presentations

Kuru, W.C., Sangalli, M., and McCready, M.J., "Onset of transverse in cocurrent gas-liquid flow." AIChE Annual Meeting, October 1995.

McCready, M., "Nonlinear stabilization of interfacial waves in fluid-fluid flows." Chemical Engineering Department, Northwestern University, May 30, 1996.

Uphold, D.D., McKee, W. and McCready, M.J., "Examination of stability models for gas-liquid flow regime transitions." AIChE Annual Meeting, October 1995.

Fundamental Processes of Atomization in Fluid-Fluid Flows

PRINCIPAL INVESTIGATOR: Prof. Mark J. McCready

University of Notre Dame

CO-INVESTIGATORS:

Chang, H.-C.

University of Notre Dame

Leighton, D.

University of Notre Dame

Task Objective:

Experiments and theoretical analysis will be used to study the detailed process involved in atomization of one fluid phase by a second shearing (continuous) phase.

Task Description:

Experiments will involve video imaging of the events leading to atomization in liquid-liquid channel and Couette flows. Eventually, data from reduced gravity gas-liquid flows will be obtained. Theoretical analysis will be comprised of analytical and numerical analysis of the Navier-Stokes equations for an evolving two-fluid interface.

Task Significance:

Droplets, formed by atomization, can enhance the mass and heat transfer between phases. Terrestrial applications include the nuclear, electric power and oil industries.

Progress During FY 1996:

The interfacial wave behavior in the Couette device has been examined in the presence of an oscillatory shear component added to steady shear. It has been observed that, usually, added oscillations are destabilizing, but for at least one set of conditions, stabilization is effected by oscillations. The theoretical work has involved constructing steady wave solutions for Couette flow waves. The predicted steady -- non steady transition is in rough agreement with experiments. Further experiments and theory are needed on this issue.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 4/96 EXPIRATION: 4/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NCC3-466

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Gallagher, C., Leighton, D.T., Chang, H.C., and McCready, M.J., Fundamental processes of atomization in fluid-fluid flows. NASA Conference Publication , 3338, pp. 89-94 (1996).

Study of Forced Convection Nucleate Boiling in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Herman Merte, Jr.

University of Michigan

CO-INVESTIGATORS:

Keller, R.B.

University of Michigan

Task Objective:

This research effort investigates the effects of buoyancy on forced convection nucleate boiling. In nucleate pool boiling, bubble detachment in normal Earth gravity is usually the result of buoyant forces; in the absence of buoyancy the bubbles have a tendency to remain in the vicinity of the heating surface, eventually causing dryout at the heating surface which results in reduced heat transfer. For boiling in a flowing liquid, an additional mechanism of bubble detachment can occur: detachment due to lift and drag on the bubble, induced by the flow field. The purpose of this study is to gain an understanding of when bubble detachment will dominate, and the effectiveness of boiling in such circumstances. Also, this study is intended to clarify the relative significance of buoyancy and bulk flow inertia forces to the critical heat flux (CHF) in forced convection boiling, which will also serve to enhance the understanding of the CHF in microgravity, where buoyancy effects are absent. This information will also increase the understanding of boiling in cases where gravity is present.

Task Description:

A closed-loop flow boiling system, using R-113 as the test fluid, has been developed. The temperature and pressure of the subcooled liquid R-113 are rigorously controlled at the entry to the test section. A portion of one wall of the rectangular test section is electrically heated to provide either a constant temperature or a constant heat flux. Surface temperature and heat flux measurements are made and the bubble growth/departure process is recorded visually. The relative effects of buoyancy are examined by rotating the entire flow loop. Other variables in the experiment are the flow velocity, the power input to the heater, and the amount of liquid subcooling.

The project has focused upon two general areas of study: obtaining heat transfer coefficients for nucleate boiling over a range of variables, and studying the conditions where dryout (departure from nucleate boiling) occurs. Analysis has been performed in both areas of study to develop physical explanations for the observed results.

Task Significance:

An understanding of the fundamentals of boiling in microgravity is necessary in order to predict the performance and limitations of space systems where boiling occurs, such as those for thermal control and power generation. Near absence of natural convection in microgravity also provides researchers the opportunity to study fundamental aspects of boiling which can improve performance of terrestrial power generation and process equipment.

Progress During FY 1996:

This study is intended to clarify the relative significance of buoyancy and bulk flow inertia forces to the critical heat flux (CHF) in forced convection boiling, which will also serve to enhance the understanding of the CHF in microgravity, where buoyancy effects are absent. Measurements of the CHF in subcooled forced convection boiling of R113 were made on a flat copper heater surface at varying orientations relative to gravity for low flow velocities, where buoyancy is substantial compared to flow forces. An analytical model describing the effects of the flow velocity, heater orientation and subcooling was developed, relying partly on empirical relationships derived from hot wire anemometer measurements of the void fraction and bubble frequency.

The experiments show that the CHF is a strong function of the heater surface orientation at very low flow velocities, and that orientation has a considerable effect on the CHF for flow velocities below 55 cm/s. In orientations where the buoyancy and flow forces oppose each other, the CHF is generally much lower than in orientations where they act in the same direction, owing to the increase in time during which the bubbles are resident at the heater surface. The analytical model of the CHF considers the motion of larger bubbles on the heater surface, relating the inverse of the bubble residence time to the CHF. The model also includes the effects of subcooling, which act to reduce the net vapor generation rate, thereby deferring the onset of the CHF to higher levels of heat flux.

In a related study, subcooled forced convection nucleate boiling experiments with R113 were conducted with thin gold film and gold coated copper substrate flat heaters. Orientation relative to gravity, flow velocity, liquid subcooling, heat flux, and heater length aspect ratio were varied to provide a better understanding of the relative roles of various heater transfer mechanisms in the total heat flux. This work was intended to better define the boiling process and determine future work for forced convection boiling in the microgravity environment of space.

The experiments and analysis demonstrated that forced convection boiling may be described by a mechanistic approach, under which the total heat flux is divided into several contributing components. A model has been developed for forced convection boiling which has an error of less than 25% for most conditions. By varying the heated length, the contributions of several of the heat transfer mechanisms were determined. Through qualitative analysis and the heat transfer model, microlayer evaporation was shown to comprise the bulk of the total heat transfer.

STUDENTS FUNDED UNDER RESEARCH:

BS Degrees: 0
MS Degrees: 2
PhD Degrees: 3

TASK INITIATION: 11/91 **EXPIRATION:** 2/96

PROJECT IDENTIFICATION: 962-24-05-68

NASA CONTRACT NO.: NAG3-131

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Brusstar, M.J., Merte, H., Jr., Effects of heater surface orientation on the CHF: Part II. A model for pool and forced convection subcooled boiling. J. Heat Mass Transfer, (1996).

Brusstar, M.J., Merte, H., Jr., Keller, R.B., and Kirby, B.J., Effects of heater surface orientation on the CHF: Part I. An experimental evaluation of models for subcooled pool boiling. Int. J. Heat Mass Transfer, (1996).

Kirk, K., Merte, H. Jr., and Keller, R.B., Low velocity nucleate flow boiling at various orientations. J. of Heat Transfer, 117, 2, pp. 380-386 (October 1995).

Proceedings

Brusstar, M.J., Merte, H., Jr., "The role of buoyancy orientation on bubble residence times and the related critical heat flux." Proc. of Symposium" Heat Transfer in Microgravity Systems," ASME HTD-Vol. 305, pp. 15-27, National Heat Transfer Conf. Portland, OR, Aug. 5-9, 1995.

A Study of Nucleate Boiling with Forced Convection in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Herman Merte, Jr.

University of Michigan

CO-INVESTIGATORS:

Dr. Lee

University of Michigan

Task Objective:

This task is a continuation of previous experimental work examining the effects of buoyancy on forced convection nucleate boiling. In nucleate pool boiling, bubble detachment in normal Earth gravity is usually the result of buoyant forces; in the absence of buoyancy the bubbles have a tendency to remain in the vicinity of the heating surface, eventually causing dryout at the heating surface which results in reduced heat transfer. For boiling in a flowing liquid, an additional mechanism of bubble detachment can occur: detachment due to lift and drag on the bubble, induced by the flow field. The purpose of this study is to gain an understanding of when bubble detachment will dominate, and the effectiveness of boiling in such circumstances. Also, this study is intended to clarify the relative significance of buoyancy and bulk flow inertia forces to the critical heat flux (CHF) in forced convection boiling, which will also serve to enhance the understanding of the CHF in microgravity, where buoyancy effects are absent. This information will also increase the understanding of boiling in cases where gravity is present.

Task Description:

A closed-loop flow boiling system, using R-113 as the test fluid, has been developed as part of a previous grant activity. The temperature and pressure of the subcooled liquid R-113 are rigorously controlled at the entry to the test section. A portion of one wall of the rectangular test section is electrically heated to provide either a constant temperature or a constant heat flux. Surface temperature and heat flux measurements are made and the bubble growth/departure process is recorded visually. The relative effects of buoyancy are examined by rotating the entire flow loop. Other variables in the experiment are the flow velocity, the power input to the heater, and the amount of liquid subcooling. A long-range goal of the effort is to adapt the current test loop for testing aboard NASA's low gravity research aircraft.

Task Significance:

An understanding of the fundamentals of boiling in microgravity is necessary in order to predict the performance and limitations of space systems where boiling occurs, such as those for thermal control and power generation. Near absence of natural convection in microgravity also provides researchers the opportunity to study fundamental aspects of boiling which can improve performance of terrestrial power generation and process equipment.

Progress During FY 1996:

The project focuses upon two general areas of study: obtaining heat transfer coefficients for nucleate boiling over a range of variables, and studying the conditions where dryout (departure from nucleate boiling) occurs. Analysis has been performed, based on related prior work, in both areas of study to develop physical explanations for the observed results.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/96 **EXPIRATION:** 7/98**PROJECT IDENTIFICATION:** 962-24-00**NASA CONTRACT NO.:** NAG3-190**RESPONSIBLE CENTER:** LeRC

Determination of Interfacial Rheological Properties through Microgravity Oscillations of Bubbles and Drops

PRINCIPAL INVESTIGATOR: Dr. Ali Nadim

Boston University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this task is to develop a complete characterization of frequency shift and damping time of the shape modes of a drop or bubble (as well as the breathing mode for the bubble) when surface transport and interfacial rheology are important.

Task Description:

Shape oscillations of bubbles and drops, freely-suspended in microgravity or acoustically-levitated on earth, have been suggested as a technique for measuring surface rheological properties as dynamic surface tension and shear and dilatational interfacial viscosities. The shape modes of an acoustically levitated drop or bubble can be excited by modulating the frequency of the ultrasound which is being used for levitation, at a frequency which is close to the natural frequency of the desired shape modes. Parameters characterizing viscous effects from the bulk phases, adsorption and desorption of soluble surfactant and their surface and bulk diffusion, the Gibbs elasticity and surface viscous effects, will all be considered and each of their contributions to the dynamics of the particular shape modes will be analyzed. The boundary integral numerical method will be extended to account for bulk viscous and diffusion effects, in an appropriate manner, using concepts from boundary layer theory for diffusion of species and momentum. The theoretical research focuses on the problems which are accessible experimentally and will aim to develop explicit procedures for obtaining the surface parameters from experimental results.

Task Significance:

Physical properties and surface rheological characteristics of materials are very important and crucial in industrial processing. Majority of these properties may be measured in a costly microgravity environment where buoyancy forces are minimized. This project introduces numerical treatment of the process to obtain these properties. Although the theoretical results of this investigation should be verified in low-gravity conditions, yet they are of great value to industrial processing, food processing, environmental protection, and pharmaceutical manufacturing as well.

Progress During FY 1996:

The PI, Prof. Ali Nadim, and his Ph.D. student, Mr. Brian Rush, have been working on this project since the summer of 1996. Advances have been made on several fronts since that time, some of which were reported in the presentation at the most recent meeting of the American Physical Society, Division of Fluid Dynamics in Syracuse, NY in November. The accomplishments include:

- (i) Calculations of the damping rates and frequency shifts for axisymmetric shape oscillations of gas bubbles with constant surface viscosity coefficients, but in the limit when the bulk fluid phases can be treated as inviscid. (These results were reported by the PI at the Third Microgravity Fluid Physics Conference sponsored by NASA Lewis during the summer of 1996.)
- (ii) Experimental work in the summer of 1996 by Mr. Brian Rush and Dr. Azuma of the National Aerospace Laboratory in Tokyo on electrically forced oscillations of flattened drops of mercury.
- (iii) Development of numerical schemes, using a spectral boundary element method, for carrying out simulations of two-dimensional drop and bubble oscillations of large amplitude.
- (iv) The quantification of the effects of bulk viscosity of the fluids on either side of the interface on the damping of drop and bubble oscillations, without surfactants.

(v) Analysis of the role of thin Stokes boundary layers near the interface of an oscillating drop on the dissipation of mechanical energy and the damping of shape modes of the drop.

The results from the above is currently being extended to the case where all effects which contribute to the damping and frequency shift of drop and bubble oscillations are taken into account simultaneously. These include dissipation in the bulk due to viscous effects, dissipation in the thin boundary layers near the interface, Marangoni effects, and surface rheology associated with surfactants. Also, the spectral boundary element method, currently developed for two-dimensional oscillations, is being adapted to treat three-dimensional axisymmetric oscillations of drops and bubbles. In addition, the effects of weak viscous damping and rheology are being incorporated into the boundary-integral method.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NAG3-184

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Brenner, H. and Nadim, A. The Lorentz reciprocal theorem for micropolar fluids. *J. Eng. Math.*, vol. 30, 169-176 (1996).

Madanshetty, S.I., Nadim, A., and Stone, H.A. Experimental measurements of shear-induced diffusion in suspension using long time data. *Phys. Fluids*, vol. 8, 2011-2018 (1996).

Nadim, A. A concise introduction to surface rheology with application to dilute emulsions of viscous drops. *Chem. Eng. Comm.*, vol. 148, 391-407 (1996).

Nadim, A., Borhan, A., and Haj-Hariri, H. Tangential stress and Marangoni effects at a fluid-fluid interface in a Hele-Shaw cell. *J. Colloid Interface Sci.*, vol. 181, 159-264 (1996).

Presentations

Nadim, A. "The role of surfactants and surface rheology in determining the rheological properties of dilute emulsions." EuroConference on Constitutive Relations and their Applications, Isaac Newton Institute for Mathematical Sciences, University of Cambridge, Cambridge, UK, April, 1996.

Nadim, A. "Shape oscillations of gas bubbles with Newtonian interfacial properties." Third Microgravity Fluid Physics Conference, NASA Lewis Research Center, Cleveland, OH, June, 1996.

Nadim, A. "Constitutive equations for dilute emulsions of viscous drops with interfacial rheology." Sixth International Conference on Discrete Methods in Fluid Mechanics, Boston University, Boston, MA, August 1996.

Rush, B.M., Nadim, A., and Azuma, H. "Nonlinear oscillations of two-dimensional drops." American Physical Society, Division of Fluid Dynamics, Annual Meeting, Syracuse, NY, 1996.

NMRI Measurements and Granular Dynamics Simulations of Segregation of Granular Mixtures

PRINCIPAL INVESTIGATOR: Prof. Masami Nakagawa

The Lovelace Institutes

CO-INVESTIGATORS:

Fukushima, E.

The Lovelace Institutes

Rosato, A.J.

New Jersey Institutes of Technology

Mustoe, G.G.W.

Colorado School of Mines

Altobelli, S.A.

The Lovelace Institutes

Caprihan, A.

The Lovelace Institutes

Task Objective:

Main objectives of this research are to develop noninvasive MRI flow measurement technique which can be used in a reduced gravity environment and to noninvasively monitor particle segregation processes using MRI. In order to conduct ground-based segregation experiments inside the limited bore space of the MRI magnet, we have designed small non-magnetic shaking and shearing devices. The basic design for the shaking box consists of two side walls and top and bottom plates. The proposed design provides enough flexibility so that any of these parts can be fixed while other parts can drive convection flow inside the box. For FY96, we manufacture a shaking box with two mobile side walls to create convection flow due to wall shear. The roughness of the inner surface of the walls may be adjusted. Once we establish steady convection flow driven by the wall(s) or plate(s), we use binary mixtures to investigate segregation of particles of different sizes due to the convection flow. Our task is to manufacture the basic shaking box and investigate the connection between mechanisms for convection flow and size segregation by noninvasive MRI measurements. In summary, our objectives are:

- 1) To build a basic shaking box,
- 2) To test the shearing box using monosize particles,
- 3) To test the shearing box using binary particles, and
- 4) To measure convection flows for monosize and binary particles using MRI.

Task Description:

Segregation experiments will be conducted using the proposed nonmagnetic shaking and shearing devices inside the limited bore space of the MRI magnet. For the ground experiments, a shaking box will be used in different configurations to investigate particle segregation due to shear induced convection flows. The shearing box with two mobile side walls as described earlier will be used first. This mode of shearing is known to produce convection flow under certain conditions of particle properties and wall conditions. We first investigate origins of wall-shear induced convection flow of single component particles by noninvasively measuring the flow and fluctuating motion of particles near rough boundaries. We then measure binary particles to identify sources for segregation.

Task Significance:

The proposed designs for small nonmagnetic (nonmetallic) shearing devices will be versatile enough to accommodate convection flow induced by different shearing motions of the boundaries under the influence of gravity. These devices will be inserted in a small bore space of the MRI magnet so that we can perform noninvasive MRI granular flow measurements. Noninvasive MRI measurements include concentration, velocity and fluctuations in velocity and they should reveal true nature of convecting flow properties and wall disturbance. A successful fabrication and instrumentation of this small MRI device will also provide possible opportunities for the fluid physics community in general to engage in non-invasive fluid flow measurements.

Progress During FY 1996:

First Quarter Progress Report:

Heug Hwan Oh, a Ph.D student, was employed to initiate granular dynamics simulations. He made modifications on the boundary conditions on our existing DEM simulation code to accommodate proposed flow driven mechanisms.

Second Quarter Progress Report:

There are three students (two undergraduate and one doctoral students) working for this project. Kevin Smith is constructing the first prototype of the shearing container. He has purchased necessary materials and prepared parts to be assembled. Jamie L. Moss is conducting experiments using a horizontal rotating cylinder until a shearing container is ready to be used. This experiment has given her an appreciation about how complex particulate flows are, especially when flows of different particles are investigated. Under the influence of gravity, for example, two different size of particles that are initially separated in two axial bands in a horizontal cylinder transform into a radially segregated structure which consists of an inner radial core containing small particles and an outer core of larger particles. We are currently investigating stability aspects of each segregation mode, radial and axial mode. This new finding further expands our research interest to investigate not only processes of segregation but also stability of segregated structures with and without the influence of gravity. Hwan Oh is working on particulate dynamic simulation. He has modified boundary conditions so that the code can simulate flows particles in a shearing box as proposed. He is also working on simulations of flows in a rotating cylinder which is also one of the proposed designs. Flows in a rotating cylinder is more directly affected by gravity and particle dynamic simulation without gravity effect should provide a valuable design guide lines.

We expect to finish the construction of a prototype shaking device by the end of January and start testing with monosize particles.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 2
MS Students: 0
PhD Students: 1

TASK INITIATION: 8/96 EXPIRATION: 8/99

PROJECT IDENTIFICATION: 962-24-00

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Nakagawa, M., Waggoner, R.A. and Fukushima, E., "NMRI measurements of flow of granular mixtures." Third Microgravity Fluid Physics Conference, Sheraton Cleveland City Center Hotel, NASA LeRC, June 13-15, 1996.

Control of Oscillatory Thermocapillary Convection in Microgravity

PRINCIPAL INVESTIGATOR: Prof. G. P. Neitzel

Georgia Institute of Technology

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective is to experimentally investigate active control of oscillatory thermocapillary convection in planar layers. The investigative strategy is as follows:

1. Establish the appropriate basic state for a "thin" rectangular flow geometry.
2. Establish and detect the oscillatory thermocapillary convection in the form of hydrothermal waves.
3. Suppression and control of the hydrothermal waves.

Task Description:

The basic state will be investigated using available computer programs to help establish the experimental design parameters and boundary conditions. After choosing the relevant design parameters and boundary conditions, the dish which will contain the desired basic state will be constructed. The desired basic state is the return flow basic state of Smith and Davis. LDV will be used to observe and measure the basic state obtained in the experiment. The surface temperature perturbations of the hydrothermal waves will then be characterized either numerically or experimentally. Control or suppression of the hydrothermal waves will be attempted using a CO₂ laser as the heat source. Locations along the free surface that appear to most effectively cancel or suppress the hydrothermal waves will be heated with a laser pulse and the duration and time of pulsing will also be compared with the predicted estimates.

Task Significance:

Crystals grown by the float-zone process can be improved by successfully suppressing undesirable fluid motion during the crystal growth process.

Progress During FY 1996:

The initial, preliminary control scheme has been shown to be effective in suppressing disturbances over several wavelengths for a handful of periods. However, since the control was previously initiated by a signal obtained from a single thermocouple embedded in the flow field through the free surface, the motion of the basic state at the free surface caused any significant disturbances induced by the CO₂ laser to be convected to the thermocouple and interrupt the control strategy. The contact of thermocouple wires with the free surface also provided an unwanted disturbance to the flow field.

The most recent work on this project has been concerned with refining the control scheme. The thermocouple has been removed from the flow field. Instead, control input is provided by signals taken directly from the infrared camera used to provide thermographic images of the disturbance temperature field during the experiment. Data are averaged along a line of length and orientation chosen by the user, the latter coinciding with the orientation of the wave fronts of observed hydrothermal waves. Frequency data determined from these spatially averaged data are fed forward to the controller for the CO₂ laser so that the controller provides laser power to the fluid along a line parallel to the hydrothermal-wave crests of the proper frequency. Results obtained are improved in the sense that the new input data appear to be much less susceptible than those provided by the embedded thermocouple to contamination provided by the heating process, allowing the suppression of waves to succeed for much longer periods of time.

Present efforts are aimed at using infrared-camera data to obtain phase speeds for the hydrothermal waves so that measured data (both amplitude and frequency) provided to the laser controller will be determined precisely for the wave being controlled. That is, the amplitude and frequency determined for a given wave will be used as the input for heating that wave, through knowledge of the phase speed of the wave and the distance between the sensing and control locations.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	3	PhD Degrees:	1

TASK INITIATION: 2/93 EXPIRATION: 2/96

PROJECT IDENTIFICATION: 962-24-05-61

NASA CONTRACT NO.: NAG3-135

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Neitzel, G.P. and Riley, J. "Control of oscillatory thermocapillary convection." Symposium on Fluids in Space, Naples, Italy, 1996.

Non-Coalescence Effects in Microgravity

PRINCIPAL INVESTIGATOR: Prof. G. P. Neitzel

Georgia Institute of Technology

CO-INVESTIGATORS:

Castagnolo, D.

MARS Center, Naples, Italy

Dell'Aversana, P.

MARS Center, Naples, Italy

Carotenuto, L.

MARS Center, Naples, Italy

Task Objective:

Non-coalescence behavior between two immiscible drops is examined. Theoretical and experimental studies will be performed which improve understanding of the non-coalescence mechanisms, identify relevant parameters that influence non-coalescence, investigate the sensitivity of the non-coalescence systems to various parameters. Drop geometries that have relevance to microgravity bearing applications will also be explored.

Task Description:

A program of experimental, theoretical, and numerical research is being undertaken to examine non-coalescence effects in liquids due to relative motion of their interfaces. An axisymmetric apparatus will be modified to study the effect of a partial vacuum. A two dimensional configuration will also be fabricated. Then non-coalescence behavior of both configurations will be explored with numerical and theoretical analyses.

Task Significance:

Potential space applications of such non-coalescing systems include: containerless confinement, shaping, and transfer of liquids. Another possible application is the development of easily formed, low-friction self-centering bearings.

Progress During FY 1996:

Progress has been made on a few different fronts. First, a two-dimensional apparatus has been designed. Fabrication of a test model was able to successfully demonstrate that non-coalescence can also be achieved in slender threads of liquid (silicone oil). Fabrication of the final version of this apparatus will be completed shortly.

Additional experiments have been performed with a drop of cylindrical symmetry in contact with a bath of liquid at a different temperature. The purpose of these experiments was to conduct further work on the development of a system for measuring the thickness of the film of lubricating gas between the liquid surfaces. This method uses an interferometric technique, creating a pattern of interference fringes whose spacing depends on the thickness of this layer. In parallel, analytical work is also being done on this front with the aim of ultimately being able to quantify the film thickness measured in this fashion. Fringe patterns created using ray tracing applied to a pair of liquid surfaces of specified shape are in very good qualitative agreement with those seen in the experiments.

Finally, work is beginning on the numerical simulation of two-dimensional, non-coalescing liquid surfaces. The problem is complicated by the disparity of length scales in the problem: liquid surfaces of size $O(10^{-3}\text{m})$ and a gas layer of thickness $O(10^{-6}\text{m})$. The initial approach will be to compute solutions for two problems. First, a global problem will be solved to determine the droplet flow fields for two droplets a specified distance apart. Results for this flow field will be used as input data to a local solution for the liquid/gas flow in the vicinity of the non-coalescing surfaces. Here, the actual deformation of the two surfaces will be computed as part of the solution.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 0

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-189

RESPONSIBLE CENTER: LeRC

Production of Gas Bubbles in Reduced Gravity Environments

PRINCIPAL INVESTIGATOR: Dr. Hasan N. Oguz

Johns Hopkins University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to provide a basic understanding of bubble formation in the reduced gravity environment by conducting experimental and theoretical studies and to develop efficient techniques of bubble production that can be readily employed by NASA. The hope is not only to provide a scientific insight into this subject but also a practical guide that will be greatly benefited by the design process of relevant processes involving small bubbles generation.

Task Description:

A good initial understanding of the processes involving bubble generation and detachment is established and there still are many issues of scientific and technological importance that need to be investigated. Two types of experiments are proposed (single bubble generation and bubble production by a compound nozzle) in addition to theoretical studies that will support the interpretation of the experimental results. Microgravity is essential for the first type of experiments in order to isolate the effects of an imposed flow on the growing bubbles. Microgravity condition is not necessary for the second type of experiments. However, such condition will be beneficial in terms of examining the details of relevant mechanisms by allowing the use of bigger jets in the experiment.

A brief description of the work to be carried out is given below:

First Year:

An apparatus for the single bubble experiment will be designed, built and used to perform the first type of experiment (single bubble generation). This will be done using Hypodermic needle in a transparent tube under normal and microgravity conditions. Water and other viscous liquids like silicon oils will be used. the goal is to understand the factors influencing bubble size and frequency in the presence of an imposed flow. Initial configuration involves using a straight tube. Other configurations involve using thick-wall needle which promotes formation of bubbles of particular size, and variable cross section tube in order to evaluate the effects of flow constrictions on the growing bubbles.

Theoretical modeling using the numerical boundary integral method simulation for inviscid and Stokes flow will be carried out. Moreover, Navier Stokes solver with viscous free surface will be initiated. Concurrently, the design for a bubble producing jet will progress and extensive tests will be performed to ensure proper operation in low gravity.

Second Year:

Possible improvements by the use of chemicals such as surfactants and coalescence inhibitors will be considered and tested. Theoretical modeling of surfactants effects will be performed. Development of Navier Stokes code will continue.

Photography will be the main measurement tool where short duration flash in conjunction with a 16 mm camera, high resolution CCD camera, high speed motion picture camera and high speed video camera will be used.

Task Significance:

In a wide variety of applications such as waste water treatment, biological reactors, flotation columns, gas liquid reactors, blood oxygenation, purification of liquids, etc. . . , it is necessary to produce small bubbles in a liquid. Since gravity plays an important role in currently available techniques, the adaptation of these applications to space will require the development of new tools. Results of this research will be beneficial for processes that require bubble generation in space. At the same time, it is anticipated that a large number of earth applications will be improved by the findings of this research.

Progress During FY 1996:

The task was initiated in the middle of July 1996. The work currently progresses in two fronts. Experiments on the bubble formation in a tube have been performed in the laboratory. Plexiglass tubes allowing clear view of the phenomenon are used in the experiments and the process have been recorded by a CCD camera in conjunction with a strobe. An undergraduate student is currently employed for this task. The theoretical work which is mostly computational, consists of (a) developing a three-dimensional potential-flow boundary-integral code and (b) adapting the front-tracking code developed by Tryggvason and co-workers to the bubble injection problem. The boundary integral code development is currently being carried out by a full time graduate student. The PI with the collaboration of Dr Takagi (Mech. Eng. Dept., U of Tokyo, Japan) is working on the Front Tracking code. Since there is no provision for the reduced gravity experiments in the approved budget the PI is currently coordinating efforts with Dr. Misawa (Mech. Eng. Lab., Tsukuba, Japan) who has access to a very high quality drop shaft facility. The experimental data will be made available to this project and compared with the numerical simulations.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/96 EXPIRATION: 7/98

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-192

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Oguz, H.N., Takagi, S., and Misawa, M., "Production of gas bubbles in reduced gravity environments." Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 13-15, 1996.

Presentations

Oguz, H.N., Takagi, S., and Misawa, M., "Production of gas bubbles in reduced gravity environments." Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 13-15, 1996.

Waves in Radial Gravity using Magnetic Fluid

PRINCIPAL INVESTIGATOR: Dr. Daniel R. Ohlsen

University of Colorado, Boulder

CO-INVESTIGATORS:

Hart, J.E.

University of Colorado

Weidman, P.D.

University of Colorado

Task Objective:

This experimental study will examine free-surface waves and their interaction with boundaries, other waves, and mean flows in spherical geometry. This geometry is motivated by comparisons to theories and idealized models as well as by applications to large-scale oceanic and atmospheric flows on the Earth and flows on the Sun and giant planets.

Task Description:

Magnetic fluid or ferrofluid is a dilute suspension of magnetic particles in a carrier fluid. In a spatially varying magnetic field, ferrofluid feels an extra body force besides normal gravity. We use magnets which make this body force nearly spherical and eliminate terrestrial gravity from the dynamics by surrounding the magnet/ferrofluid structure with immiscible fluid of the same density. Waves are then driven on the ferrofluid surface with external magnets.

We will examine capillary-gravity waves on both the full spherical surface and within channels and basins on the sphere. An equatorial channel is a straight wave tank which is truly periodic in the downstream direction and allows direct comparison for the first time to theoretical and computational models which often make this assumption. The addition of overall rotation to the system allows planetary waves to be studied.

Ferrofluid is black and opaque so waves can be detected on a free surface in profile. A scanning profiling system is under development for imaging of the full spherical surface. Ultrasound and/or magnetic induction-based techniques will be tested for detection of internal motions, particularly for stratified experiments.

Task Significance:

Waves on a fluid with a free surface subject to radial gravity on a sphere is the canonical setup for studies of some of the large-scale dynamics of the Earth's ocean and atmosphere as well as the giant planets and the Sun. This experiment is significant because these elements have not been simultaneously possible in laboratory experiments before. The experiments will provide ground-truth data for comparisons to large computer simulations of the atmosphere and ocean. A missing element remains density variations owing to stratification or thermal forcing. These ground-based experiments should demonstrate whether adding this element, requiring the microgravity environment, is feasible and scientifically justified.

Progress During FY 1996:

1. Construction of the initial permanent magnet version of the experiment is nearly complete. We have changed to an oil-based ferrofluid in order to avoid the use of large quantities of freon fluid which has become unavailable.
2. A research associate has been hired to begin this Fall on the project.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-184

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Ohlsen, D. R., Hart, J. E., and Weidman, P. D., "Waves in radial gravity using magnetic fluid." Third Microgravity Fluid Physics Conference, NASA Lewis Research Center, Cleveland, OH, June, 1996..

Industrial Processes

PRINCIPAL INVESTIGATOR: Prof. Simon Ostrach

Case Western Reserve University

CO-INVESTIGATORS:

Kamotani, Y.

Case Western Reserve University

Task Objective:

The objectives of this study are to gain an understanding of the role of gravity in various industrial processes and to develop new applications of microgravity.

Task Description:

The commercial processes and related basic processes which have been investigated or are being investigated, include supercritical extraction processes, coating flows, formation of bubbles in liquid flow, dynamics of liquid-gas interfaces, transport phenomena in zeolite growth, rotating electrochemical systems, and transport phenomena in crystal growth. The roles of gravity in those processes are being studied by using experimental, numerical, and analytical techniques and potential benefits of microgravity are being assessed. Based on those studies microgravity experiments will be proposed.

Task Significance:

The roles of gravity in terrestrial and space-based industrial processes are being studied by using experimental, numerical, and analytical techniques, and the potential benefits of microgravity applications of these processes are being assessed. Based on these studies, microgravity experiments will be proposed which will lead to an understanding of how to best utilize the environment of space for various industrial applications.

Progress During FY 1996:

1. Coating Flows:

Experimental work on coating flows has been written as a Ph.D. thesis and numerical analysis is continuing.

2. Bubble Generation in Microgravity:

Preliminary ground-based experiments have been conducted on bubble generation in a flowing liquid medium. A DC-9 rig has been constructed for reduced gravity tests at LeRC.

3. Rotating Electrochemical Cells:

Experiments to measure mass transfer rates in rotating systems have been completed. Numerical analysis to obtain more information above the velocity fields has also been completed. This work has been written as a Ph.D. thesis.

4. Natural Convection in Circular Cylinders:

An experiment on oscillatory natural convection of a low Prandtl number fluid in circular cylinders has been completed and written as a Ph.D. thesis.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 1/89 EXPIRATION: 3/96

PROJECT IDENTIFICATION: 962-24-05-30

NASA CONTRACT NO.: NAG3-886

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Jiang, H.D., Kam, V., Kamotani, Y. and Ostrach S., Transport phenomena in supercritical fluid extraction. Chem. Eng. Comm, vol. 132, (October 1995).

Jiang, H.D., Ostrach, S., and Kamotani, Y., Thermosolutal transport phenomena in large lewis number electrochemical systems. International Journal of Heat and Mass Transfer, (1996).

Presentations

Ostrach, S., Kamotani, Y., "Industrial processes influenced by gravity." Third Microgravity Fluids Physics Convergence, June 13-15, 1996.

Selver, R., Kamotani, Y., and Ostrach, S., "Natural convection of a liquid metal in vertical circular cylinders heated locally from side." Accepted for presentation at ASME IMECE, 1996.

Industrial Processes Influenced by Gravity

PRINCIPAL INVESTIGATOR: Prof. Simon Ostrach

Case Western Reserve University

CO-INVESTIGATORS:

Kamotani, Y.

Case Western Reserve University

Task Objective:

The objective of this study is to investigate gravity dependent transport phenomena in various industrial processes in order to indicate new directions for microgravity research that enhances the commercial success of the space program. The underlying and unifying basis for the present study is the biophysicochemical transport phenomena which are modified by gravitational forces. The important implications include the effects of fluid flow, head and mass transfer on biology and chemical reactions. Inversely, the transport phenomena associated with such processes are different in a modified gravitational environment.

Task Description:

The present research effort is ground-based. We have identified various industrial processes for applications in space. In particular, the present research focuses on the following subjects: The first subject is a study of rotating electrochemical systems directed towards the understanding of the transport phenomena in rotating nickel-zinc (Ni-Zn) battery system. The second task is a study of coating flows motivated by the desire to understand the transport phenomena in industrial coating processes. The third subject is study of convection in low Prandtl number fluids in order to understand the transport phenomena during crystal growth.

In the rotating battery work we investigate, experimentally and numerically, the solutal convection inside a shallow rotating electrochemical cell with concentration differences between two electrodes. A dilute binary electrolyte, cupric-sulfate system is the working fluid in both experimental and numerical simulations. The limiting current method is used to measure the mass transfer rate in the cells. The numerical analysis is limited to cases when the flows is axisymmetric and laminar. The basic equations with their appropriate boundary conditions are discretized and solved by the SIMPLEC scheme.

Coating processes require the final film thickness to be very thin and highly accurate. Also, for productivity reasons they strive for high speed applications and several discrete film layers are at times applied simultaneously. As a result of such demands, attempts to use a specific coating process for a given application frequently fail. The liquid layer may not be continuous and, if it is, waves or streaks may occur. Using both numerical and experimental methods we show that the final film in microgravity can be made smoother and much thicker.

Since semi-conductor crystals are a very important component of the electronic industry, it is worthwhile to seek a control strategy that will lead to the reduction of periodic inhomogeneities. The present work presents the detailed physics of the transport phenomena in a liquid metal in vertical cylinders which are designed to simulate the zone-melting crystal growth technique. The main focus is on oscillatory natural convection. The conditions for the onset of oscillations and the oscillatory flows are investigated.

Task Significance:

The present study is directed to understand the transport phenomena in industrial processes and to develop a knowledge base for their applications with emphasis to a microgravity environment. The main motivation comes from the fact that transport phenomena influenced by gravity are a vital element of the chemical, pharmaceutical, energy production, material processing and biotech industries. The present results demonstrate a great potential for space applications. The present study on the transport phenomena in rotating electrochemical systems is beneficial to an optimal design of rotating batteries. The optimal performance of a coating device at a high parametric range is shown to be hindered by gravity and the final film becomes wavy. The present study reveals the nature of the waves and maps the undesired parameter range although more work is needed to confirm the cause of the wavy motion. In the study of convection of a liquid metal in vertical cylinders, the measurement of the amplitude and phase of temperature traces at different azimuthal position reveals oscillatory convection, which has important implications to crystal growth from melts.

Progress During FY 1996:

The experimental mass transfer results obtained in the rotating electrochemical cell are found to agree well with the scaling law we derived earlier. The present numerical work analyzes the flow structure and the concentration distribution. It is found that at relatively low rotation speed the core flow is mainly unicellular. The unicellular flow is sandwiched between two Ekman layers along the top and bottom walls. When the rotation speed exceeds a critical value or when the Ekman number is less than certain value, a series of secondary flow cells appear in the core region. The secondary flow is induced by the Coriolis force. The multiple flow cells mainly occur in the core region, hence their influence on the mass transfer rate is weak. Also, it is shown that the centrifugal buoyancy force enhances the mass transfer rate to the electrodes. The present results show that it is possible to control and stabilize the shape-change effects in Ni-Zn batteries, which leads to an increase in the charging and discharging life cycle and gives high specific power.

The coating flow experimental and numerical data indicate that gravity significantly influences the stability of a coating film. The coating film exhibits an interfacial instability beyond a certain Reynolds number and becomes wavy. The non-dimensional parameters that influence the coating flow were derived. The present study depicts the following trends: First, when the Reynolds number (Re) is small, the non-dimensional film thickness becomes constant beyond a certain capillary number. Second, when Re is large, the film thickness depends on the Weber number (We) and Re. Beyond about $We=0.2$ the final film thickness becomes constant, independent of We and Re. Also the present study reveals that when the relative Re exceeds unity, a dip coating film becomes unstable. The film meniscus shape is investigated using both numerical and experimental techniques. The numerical results are obtained using a Fluent Nekton code.

The study on convection in low Pr fluids covers a wider range of Ar (aspect ratio) than those used in the crystal growth technique in order to study oscillatory convection under more general conditions. Thermocouples are placed at different azimuthal positions along the wall to detect the onset of oscillations and to determine the oscillation flow structures and frequencies. The values of critical Rayleigh number for the onset of oscillation are measured under various conditions. The temperature oscillation pattern and the corresponding frequency are also due to a thermal instability and the oscillation are due to the fact that the unicellular motion is rotating back and forth. When Ar is below 6, the oscillation pattern is associated with a rotation non-axisymmetric toroidal pattern around the axis.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	3	PhD Degrees:	1

TASK INITIATION: 3/96 EXPIRATION: 2/97

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NAG3-186

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Kizito, J. P., Ostrach, S., and Kamotani, Y., "Free coating flow at high capillary and Reynolds numbers." Ph.D. Thesis, Case Western Reserve University, Cleveland, 1995.

Selver, R., Kamotani, Y., and Ostrach, S., "Natural convection of a liquid metal in vertical cylinders heated locally from side." Presented at the 1996 ASME International Congress and Exposition, Atlanta, 1996.

Marangoni Effects on the Bubble Dynamics in a Pressure Driven Flow

PRINCIPAL INVESTIGATOR: Prof. Chang-Won Park

University of Florida

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The main objective of this study is to investigate the surfactant-induced Marangoni effects on the motion of bubble drops in Hele-Shaw cell.

Task Description:

Experiments are conducted using water drops containing a pre-determined amount of surfactant. The transnational velocities of the water drops in an oil-filled Hele-Shaw cell are measured and the shape evolution of the drops are observe.

Task Significance:

Surface active substances, which are often present as contaminants, are known to have significant influence on the motion of bubbles and drops. The present study investigates the surfactant influence quantitatively using a model system. This study has a close relationship to a number of multi-phase fluid systems in the area of materials processing, direct contact mass and heat transfer devices, and bioengineering which has direct implication for space-based applications.

Progress During FY 1996:

The experiments with fluorocarbon oil drops have shown a agreement with the predictions of Taylor-Saffman theory for surfactant-free drops. Water drops, on the other hand, have shown significant retardation (by an order of magnitude compared to the TS theory). This difference is due to the fact that an oil-oil interface is not prone to the influence of surface active substances whereas an oil -water interface is, even though surfactants are present in both cases.

A theoretical calculation for an elliptic bubble predicts the transitional velocity of the bubble as a function of capillary number. While the Taylor-Saffman result is recovered when the bubble surface is surfactant-free, a significant retardation is predicted in the presence of surfactant. This prediction is apparently in agreement with the experimental observations.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/94 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-24-05-92

NASA CONTRACT NO.: NAG3-163

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Maruvada, S.R.K. and Park, C.-C., Retarded motion of bubbles in Hele-Shaw cells. Phys. Fluids, (1996).

Presentations

Maruvada, S.R.K and Park, C-W., "Retarded motion of bubbles and drops in Hele-Shaw cells." Annual meeting of AIChE, Miami, FL, November 1995.

Maruvada, S.R.K and Park, C-W., "Retarded motion of bubbles and drops in Hele-Shaw cells ." 48th Annual meeting of the Division of Fluid Dynamics, American Physical Society, Irvine, CA, November 1995.

Nonlinear Dynamics and Nucleation Kinetics in Near-Critical Liquids

PRINCIPAL INVESTIGATOR: Prof. Alexander Z. Patashinski

Northwestern University

CO-INVESTIGATORS:

Ratner, M.A.

Northwestern University

Pines, V.

Case Western Reserve University

Task Objective:

The objective of this theoretical research is to develop a more complete understanding of the nonlinear response of a near-critical liquid to strong perturbations of local thermodynamic equilibrium. The consideration is limited to a set of special physical situations relevant to flight experiments dealing with relaxation and nucleation in a near-critical state. It entails the hierarchical relaxation in a macroscopically homogeneous non-equilibrium liquid following homogeneous strong, rapid temperature, and pressure perturbations of thermodynamic equilibrium, interaction of such perturbations with inhomogeneities, their influence on nucleation kinetics, and the kinetics of a sub-critical nucleus.

Task Description:

The general theoretical method is the field theory approach to near-critical systems, the scaling theory of critical phenomena, and computer simulations.

One physical situation to be theoretically studied is described in the form of idealized experiments. This situation includes temperature changes in a near-critical liquid at time scales shorter than the relaxation time of correlated fluctuations. The behavior of a nucleus near the phase separation line in non-stationary temperature conditions will be examined in order to find the way for direct observation of a sub-critical nucleus.

The expected results of the theory are new scaling laws for the long-time dependence of the temperature and for the statistical characteristics of long-range fluctuations. These predictions may be tested in microgravity conditions by light scattering and direct visualization experiments.

The relaxation of a non-equilibrium near-critical system following strong rapid perturbations is expected to yield conditions for achieving a near-critical steady state with a constant heat current and to formulate optimal conditions for a potential flight experiment.

Task Significance:

The study of the response of an equilibrium near-critical liquid to rapid perturbations is expected to give insights into phenomena accompanying such perturbations in experiments very close to the critical point, including already performed flight experiments. The computer study of the nucleation allows one to compare the slow kinetics of nucleation in a near-critical fluid with the nucleation in technologically important conditions.

Progress During FY 1996:

This work came to a close in June 1996. The work concluded with renormalization analysis of slow and rapid temperature steps separately towards and away from the critical point from an initial homogeneous state. Two publications listed cover this in detail. The work describes the different relaxation behavior when the temperature change requires transformation from short-range correlations to long-range correlations versus transformation from long-range correlations to short-range correlations.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/94 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-24-05-07

NASA CONTRACT NO.: NAG3-161

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Mitus, A.C., Smolej, F., and Patashinski, A.Z., Q446 <Shape Spectroscopy> of local f.c.c. structures in computer simulations of crystallization. Europhysics Letters, vol. 32 (9), p. 777 (December 20 1995).

Patashinski, A.Z., One temperature step away from the critical point. Physical Review E, vol. 54 (3), p. 2479 (September 1, 1996).

Patashinski, A.Z., Rapid temperature changes near a critical point. Physics Letters A, vol. 219 (1/2), p. 131 (August 12, 1996).

Patashinski, A.Z. and Ratner, M.A., Orientation relaxation in glassy polymers. II. Dipole-size spectroscopy and short-time kinetics. The Journal of Chemical Physics, vol. 103 (24), (December 22 1995).

Two-Phase Interfaces in Weak External Fields

PRINCIPAL INVESTIGATOR: Prof. Jerome K. Percus

New York University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The aim of this work is to understand from first principals the behavior of two-phase interfaces in the absence of assumptions as to gravitational effects.

Task Description:

1. Analytical Statistical Mechanical formalisms will be employed. Classical Hamiltonians of the interfaces of interacting fluids will be modified or developed as needed.
2. General external fields are included.
3. Equilibrium, followed by non-equilibrium, descriptions are to be employed. It is expected that familiar and new strategies will be utilized.

Task Significance:

The above objective is fundamental to our ability to deal with the fluid structures that abound in the real biological, chemical, and physical world.

Progress During FY 1996:

Study continued on the interaction energy between droplet surfaces at very close separation in a vapor environment. This is crucial to the dynamics of condensation from over-saturated vapor and requires close control of the surface fluctuations. Initial work has been focused on a model in which the liquid/vapor density ratio is very high, typical of fluids such as water well below the critical point. A number of technical issues have to be met, notably that of determining the properties of fluctuations that are Gaussian but over a restricted space.

NASA funding for this work concluded after 5 months of this FY.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 1/93 EXPIRATION: 3/96

PROJECT IDENTIFICATION: 962-24-05-76

NASA CONTRACT No.: NAG3-141

RESPONSIBLE CENTER: LeRC

On the Boundary Conditions at an Oscillating Contact Line: A Physical/Numerical Experimental Program

PRINCIPAL INVESTIGATOR: Dr. Marc Perlin

University of Michigan

CO-INVESTIGATORS:

Schultz, W.

University of Michigan

Task Objective:

The primary goals of this research program are to provide a physical explanation of oscillatory contact-line behavior, a more accurate boundary model for large-amplitude (high Reynolds number) oscillations, and an attempt to model dissipation in the vicinity of the contact line.

Task Description:

The multifaceted effort will include precision experiments, analytical modeling, and numerics. Being a first year effort, a more detailed outline of the specific tasks is provided below.

Task Significance:

While in terrestrial flows the body force attributable to gravity is expected to be locally unimportant, the local behavior of the capillary surface in the near vicinity of the moving contact line may dominate the flow. Knowledge gained from such an investigation is valuable to in-space fluids management and is essential to the design and prediction of system performance (i.e. partially-filled reservoirs in the microgravity environment, liquid fuel, oxygen tanks, etc.). The understanding of nonlinear fluid oscillation and damping is a particular concern to long duration space flight missions.

Progress During FY 1996:

The specific objectives of this research are: (1) to conduct precise, high-resolution measurements of the flow field in the immediate vicinity of the contact line and as a function of position along a vertically oscillating vertical plate using particle-image-velocimetry techniques (These measurements are conducted either along a vertically oscillating upright plate partially immersed in a reservoir, or along the wall of a vertically oscillating reservoir in which Faraday waves exist. Our preliminary experience with Faraday waves, Jiang, et al. 1996a and Jiang, et al. 1996b, has shown that the waves are "cleaner" than those produced by vertical or horizontal oscillation of walls. They are easier to model analytically and computationally, and they do not have strong vortex formation at the bottom of the plate.); (2) to compare the measured velocity fields with those predicted by the exact analytic solution (for laminar flow) of Stokes, thus defining the slip region as well as elucidating the effect of the contact line, meniscus, and the interface on the local fluid physics, this by investigating the deviation from the exact solution; (3) to develop a proper boundary condition for the stick-slip motion of the contact-line region (Ting and Perlin, 1995 did not include the effects of acceleration directly); (4) to develop a numerical code to simulate the flow field using the boundary condition developed and the viscous equations of motion; and (5) to verify and quantify the accuracy of the boundary conditions developed by comparing the interfacial elevations and flow fields of the measurements with those of the numerics. Dissipation, the size of the eddy near the contact line, and hysteresis are measured and compared to linear and nonlinear models of viscous and (when appropriate) irrotational models.

Measurements and numerics are compared in detail. We have a "closed-loop" prediction in the sense that our experiments determine boundary conditions along the plate. We generate numerical solutions with these boundary conditions and finally compare the flow field adjacent to the plate with the flow field calculated numerically to quantify and verify the applicability of our boundary conditions.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-186

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Jiang, L., Perlin, M., and Schultz, W.W., Breaking faraday waves. 21st ONR Sym of Naval Hydro, Trondheim, NOR, (1996).

Jiang, L., Ting, C.-L., Perlin, M., and Schultz, W.W., Moderate and steep Faraday waves: instabilities, modulation and temporal asymmetries. *Journal of Fluid Mechanics*, (1996).

Ting, C.-L. and Perlin, M., Boundary conditions in the vicinity of the contact line at a vertically oscillating upright plate: an experimental investigation. *Journal of Fluid Mechanics*, vol. 295, 263-300 (October 1995).

Fluid Dynamics and Solidification of Molten Solder Droplets Impacting on a Substrate in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Dimos Poulikakos

University of Illinois, Chicago

CO-INVESTIGATORS:

Megaridis, C.M.
Vedha-Nayagam, M.University of Illinois at Chicago
Analex Corporation

Task Objective:

The objective of this program is to investigate the fluid dynamics and simultaneous solidification of molten solder droplets impacting on a flat surface. The problem is directly relevant to the printing of microscopic solder droplets during surface mounting of microelectronic devices. The study will identify the degree of influence of the dominant process parameters on specific aspects of solder droplet dispensing. The data produced will be analyzed to define the domains of solder microdroplet dispensing operational parameters that result in optimal and consistent production of solder bumps as needed for specific industrial applications.

Task Description:

The study consists of a theoretical and an experimental component. The theoretical work uses computer models based on finite element techniques. The experimental work is performed in microgravity in order to allow for the use of larger solder droplets that make feasible the performance of accurate measurements while keeping the effect of gravity negligible.

Task Significance:

The technology of solder microdroplet dispensing has shown great promise in microelectronic packaging and assembly. Therefore, the development of a good understanding of the pertinent fluid dynamics and solidification phenomena is essential for the successful commercial implementation of the technique. Conducting experiments in microgravity eliminates the unwanted influence of gravity and makes the experimental investigation of large droplet dispersion directly relevant to the actual application where solder droplets are approximately four thousands of an inch in diameter.

This program will advance the state of knowledge and provide a science base for the fundamental transport phenomena occurring in the novel solder microdroplet dispensing technology. The study will also provide predictive tools to be used for the successful development, and eventually, commercialization of this innovative technique in electronic component manufacturing or other relevant technologies. If successful, this effort is expected to have a significant impact on establishing solder microdroplet dispensing as the process of choice among electronic packaging manufacturers.

Progress During FY 1996:

This is a new task (commenced on 6/96).

STUDENTS FUNDED UNDER RESEARCH:BS Students: 2
MS Students: 1
PhD Students: 1

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-190

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Poulikakos, D., Megaridis, C. M. and Vedha-Nayagam, M., "Fluid dynamics and solidification of molten solder droplets impacting on a substrate in microgravity." Presented at the Third Microgravity Fluid Physics Conference, Cleveland OH, June 13-15, 1996.

Acoustic Bubble Removal from Boiling Surfaces

PRINCIPAL INVESTIGATOR: Prof. Andrea Prosperetti

Johns Hopkins University

CO-INVESTIGATORS:

Oguz, H.
Trinh, E.I.Johns Hopkins University
Jet Propulsion Laboratory (JPL)**Task Objective:**

The objective is to investigate the effectiveness of acoustic means to remove vapor bubbles generated at a boiling surface, and thus enhance boiling heat transfer in low gravity.

Task Description:

Acoustic effects considered for effective heat removal include the following: The bubble resonance due to the vapor bubble stiffness, the bubble resonance due to surface tension, the force on the bubble due to pressure radiation, and the effect of steady streaming flows due to the interaction of acoustic waves and the walls and the vapor bubbles.

Theoretical and experimental work is planned to study these mechanisms to improve boiling heat transfer. 1-g experiments will be carried out to test these concepts.

Low-gravity tests (DC9) will be undertaken to refine the ground-based research.

Task Significance:

At normal gravity, a major portion of the effectiveness of saturated boiling as a heat transfer mechanism is due to the fact that buoyancy continuously removes bubbles from the heated surface. In space one cannot rely on this mechanism. The purpose of these experimental and theoretical studies is to explore a wide range of acoustic effects as potential means to substitute for the missing buoyancy force.

Progress During FY 1996:

This is a new grant starting in FY96. One post-doctoral researcher has started numerical investigations pertaining to the two linear resonance frequencies of the vapor bubbles; extension of this work to non-linear analyses is in progress. The results to date was presented at the American Physical Society Fluid Dynamics Division meeting (November 24-26, 1996), and at the Acoustical Society of America meeting (December 2-6, 1996).

STUDENTS FUNDED UNDER RESEARCH:BS Students: 0
MS Students: 0
PhD Students: 1.5

TASK INITIATION: 7/96 EXPIRATION: 7/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-192

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Prosperetti, A. and Oguz, H.N., "Acoustic behavior of vapor bubbles." Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 13-15, 1996.

Containerless Ripple Turbulence

PRINCIPAL INVESTIGATOR: Dr. Seth J. Putterman

University of California, Los Angeles

CO-INVESTIGATORS:

Barmatz, M.
Meyer, W.California Institute of Technology
NASA Lewis Research Center (LeRC)

Task Objective:

We are working toward the goal of studying turbulence in a broad-band spectrum of capillary waves that run around the surface of a containerlessly positioned drop of liquid. This experiment would constitute the first controlled measurement of turbulence in interacting waves.

Task Description:

The problem consists of two components. They are (a) the generation of a turbulent distribution of surface ripples and (b) the detection and measurement of this state. These issues are being approached in ground-based experiments as well as in arrangements that simulate containerless fluids in microgravity. The ground-based experiments are being carried out in a fluid which is excited with a shake table. The preflight experiments are being developed with a levitated droplet of liquid.

Task Significance:

Consequences of this experiment range from the characterization of turbulence to the determination of universal properties of nonlinear systems and signal processing. The presence of a new propagating mode (second sound) in the capillary turbulence would have important ramifications with regard to attempts to achieve controlled thermonuclear fusion.

Progress During FY 1996:

- 1) We have excited high amplitude surface waves which demonstrate a transition to turbulence.
- 2) We have developed a new imaging technique which enables us to measure instantaneously the surface height as a function of position for high amplitude motion.
- 3) We have developed tools for data analysis that enables us to:
 - a) Measure the frequency and wave number dependence of turbulence and
 - b) Elucidate structures (i.e. intermittency) in the midst of the turbulent motion.

Note: Our laboratory is the only lab capable of making quantitative measurements of intermittence in turbulence.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-188

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Wright, W.B., Budakian, R., and Putterman, S.J., Diffusing light photography of fully developed isotropic ripple turbulence. *Physical Review Letters*, vol. 76, 4528-4531 (June 10, 1996).

Proceedings

Wright, W.B., Budakian, R., and Putterman, S., "Resolving high amplitude surface motion with diffusing light." *Proceedings of the 3rd Microgravity Fluids Conference Proceedings*, NASA Lewis Research Center, R. Ziegfeld ed., June 13-15, 1996.

Decoupling the Role of Inertia and Gravity on Particle Dispersion

PRINCIPAL INVESTIGATOR: Dr. Chris B. Rogers

Tufts University

CO-INVESTIGATORS:

Squires, K.

University of Vermont

Pothier, S.

Delta Airlines

Task Objective:

Our primary objective in this work is to determine the influence gravitational forces play on the behavior of small solid particles in air. Particle behavior is dictated by particle inertia, particle weight, and local fluid turbulence. By placing particles in a decaying isotropic fluid field in a zero-gravity environment, we will be able to measure the role inertia plays in particle dispersion and response to fluid turbulence.

Task Description:

Our goal is to isolate the effects of gravity on particle behavior. We will do this by measuring particle dispersion and velocity in a zero-gravity, simple turbulence fluid environment. We will make these measurements by using two (stereo) video cameras and tracking individual particles in time. The whole apparatus will be flown on the NASA research aircraft to simulate a zero-gravity environment. From these dispersion measurements, we will be able to better model how different particles react to their surrounding turbulence.

Task Significance:

Air flows with small solid particles are common throughout industry, from paint spraying to paint removal, from dust-free rooms to contaminant control. Nature, too, provides many such flows - the most dramatic being volcanic explosions and dust storms. How these particles actually move, however, is difficult to predict. These particles will respond to the fluid turbulence they experience as they move through the air. Similar to a jet aircraft in atmospheric turbulence, these particles respond to the turbulence along their path: a path influenced by their inertia and by their weight. Heavier particles will tend to be pulled through turbulence faster than their lighter counterparts; thus having less time to react. Particle inertia, too, makes a difference. The 747, for instance, will not be as bumpy as the smaller 737 aircraft. However, since the particles have no propulsion mechanism of their own, large inertia particles corresponds to heavier particles - making it difficult to discern inertial from gravitational effects. This complicates modelling of particle behavior. By examining particle response in a zero-gravity environment, we are able to look specifically at inertial effects. Therefore, although the main goal of this research is to better understand and model the fundamental physics behind particle behavior, its results will have direct applicability to a number of different industrial and natural occurrences. Further, the results of this work will be critical to understanding particle behavior in future space-based applications, from manufacturing to combustion.

Progress During FY 1996:

Since the program's initiation two months ago, we have:

- Developed an initial tunnel design with a fully working water-based prototype
- Developed the necessary fluid diagnostic software (PIV)
- Started development on the 3-D tracking software (SIV)
- Uploaded to Tufts an existing Direct Numerical Simulation (DNS) of isotropic turbulence and ran some simple cases (Squires's code from UVM)
- Began development on a new DNS code to take advantage of multi-processors
- Met with NASA project manager and defined limitations of both drop-tower and research aircraft experiments.

By the end of the first year, we plan on testing a working air-base experiment on a private aircraft at Tufts. We also plan to have a working particle tracking system along with extensive mapping of the fluid turbulence through our PIV system.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 4

PhD Students: 0

TASK INITIATION: 6/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NCC-3-47

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Rogers, C.B. and Squires, K.M., "Decoupling the role of inertia and gravity on particle dispersion." Microgravity Meeting, 1996.

Studies of Radiation-Driven and Buoyancy-Driven Fluid Flows and Transport

PRINCIPAL INVESTIGATOR: Prof. Paul D. Ronney

University of Southern California

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The proposed research will consist of two sets of experiments under simulated microgravity condition. The first is a study of instabilities of radiating, initially-homogeneous gas volumes, for both optically-thin and optically-thick gases with a vertical temperature gradient between two plates. The objectives are to determine the validity of theoretical stability criteria and to determine the spectrum of the nonlinear evolution of the resulting densifications. The second set of experiments is a study of the stability of one-dimensional steady temperature profiles and unsteady thermal conduction waves in gases with strongly temperature-dependent radiative conductivity. The objective is to determine the stability criterion, study nonlinear evolution's of these instabilities, and develop a stability model.

Task Description:

The following are proposed problem studies:

1. Stability of a cooling optically-thin gas volume (field instability) using NH_3 gas condensable I_2 vapor or other gas with analogous properties, and measurement of the power spectrum of any resulting nonuniformities.
2. Stability of a cooling optically-thick gas volume which is opaque only at high temperatures (CMBR instability) using CO or other gas with analogous properties, and measurement of the power spectrum of any resulting nonuniformities.
3. Radiative conduction in optically-thick gases between parallel plates using SF_6 .
 - a. Radiatively-induced instabilities of steady planar conduction profiles at μg .
 - b. Unsteady planar conduction at constant heat flux (thermal waves) at one-g and μg .
 - c. Critical Rayleigh numbers at one-g at large t and ΔT .
4. Radiative conduction in optically-thick gases at μg in spherical geometry.
5. Theoretical stability analysis corresponding to items 3 and 4.

Task Significance:

The study of the coupling of internal radiation to fluid flow is important in a wide variety of practical problems including glass and semiconductor processing; oceanographic, atmospheric and astrophysical flows; plasma physics; combustion systems; solar energy collection; and heat transfer in inhabited enclosures. This work consists of a series of experiments to be carried out in the drop towers that will enhance the understanding of the physics of internal radiation to fluid flow. Results obtained from the present research could identify potential mechanisms to improve the Earth's environment and improve solar power systems.

Progress During FY 1996:

This year, the drop test rig has been redesigned to provide a total of 800 Watts to the heating/cooling systems. Ground-based tests, as well as drop tests indicate that there is sufficient power to maintain the plates at the desired temperatures for up to 20 minutes.

The Rayleigh-Benard apparatus was altered to provide a greater temperature difference between the plates. Several additional heating elements were added to raise the maximum temperature of the hot plate. Correspondingly, the heat removal system of the cold plate was also expanded.

Second and third drop campaigns were completed this year. Gas-phase thermocouples and a narrow-angle radiometer were added to the Rayleigh-Benard apparatus with the intent of characterizing the flows observed in previous drop tests. Flow induced by buoyancy prior to drops was virtually eliminated via the use of carefully placed baffles and insulation. The results produced much new information regarding the presence of radiative energy fluctuations throughout the medium tested.

In agreement with previous tests, flows were observed at higher temperatures and pressures. Tests conducted with SF₆ at 2 atm or greater yielded flows with velocities similar to those already observed. The thermocouple measurements taken indicated temperature fluctuations as well as an increase in the overall temperature of the test region. The fluctuations were large relative to the minor fluctuations observed in 1 g tests under the same conditions.

Data from the radiometer denoted large fluctuations in radiant energy as well as an overall increase in energy throughout the duration of the SF₆ tests. No such fluctuations were present in any N₂ experiment. Using SF₆, the highest level of fluctuations occurred in drops where the temperature difference between the plates was greatest.

This suggests an advantage to supplying an even greater temperature difference between the plates for further experiments. An additional radiometer and two thermocouples are currently being added to the apparatus for future tests. A fourth drop campaign has been scheduled for September to further characterize the flows observed in the SF₆ and CO₂ tests.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 0

TASK INITIATION: 6/94 **EXPIRATION:** 6/96

PROJECT IDENTIFICATION: 962-24-05-93

NASA CONTRACT No.: NAG3-165

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Fortmeyer, J.M. and Ronney, P.D., "Radiatively-driven flows in gases." 48th Annual Meeting, Division of Fluid Dynamics, American Physical Society, Irvine, CA., November 19-21, 1995.

Fortmeyer, J.M. and Ronney, P.D., "Studies of radiation-driven and buoyancy-driven Fluid flows and transport." Third International Microgravity Fluids Workshop, NASA LeRC, Cleveland, OH., June 13-15, 1996.

Fluid Creep Effects on Near-Wall Solute Transport for Non-Isothermal Ampoules and Suspended Particle Transport Coefficients

PRINCIPAL INVESTIGATOR: Prof. Daniel E. Rosner

Yale University

CO-INVESTIGATORS:

Papadopoulos, D.H.

Yale University

Task Objective:

One goal of this proposal is to initiate theoretical studies necessary to provide the basis for more realistic future ampoule-level numerical simulations for multi-component vapor transport, including supercritical vapors. A second goal is to provide predictions of particle (or macro-molecule) transport properties based on similar phenomena occurring at the particle level.

Task Description:

This research program was focused on the formulation/consequences of appropriate fluid/solid boundary conditions (BCs). Having pointed out the importance of non-isothermal wall-induced gas creep phenomena in microgravity (and even ground-based) crystal growth experiments, theoretical studies have been formulated and carried out which provide a firm basis for more realistic future ampoule-level numerical simulations for vapor transport/crystal growth. Opportunities for flight experiments to obtain reliable data on such BCs have been pointed out.

The following are issues to be addressed in this investigation:

- (1) Slip coefficients for polyatomic gases, including nondilute, disparate molecular weight mixtures.
- (2) Simultaneous effects of wall creep due to solute mass-transfer, including the coupling between creep associated with energy and mass transfer.
- (3) Nature of the transition from the Enskog-Chapman regime to the case of liquid-like densities.
- (4) Appropriate "creep" conditions at "porous" solid surfaces; implications for the transport properties of suspended particles, including thermophoretic coefficients.

Task Significance:

These phenomena not only influence transport rates in microgravity crystal growth ampoules, but also the migration rates of suspended macromolecules or nanoparticles (molecular clusters and ultra fine particles).

Progress During FY 1996:

The feasibility of applying a microscopic approach based on the Boltzmann equation for low-density gases to the 'model' problem of thermal creep in a two-dimensional ampoule with strong temperature gradients established along its side-walls was investigated early on. Toward this end, a Direct Simulation Monte Carlo (DSMC) method was selected which was based on the algorithm proposed by G. Bird (1994). For simplicity, the geometry chosen is a cartesian one. The code for this purpose has been developed and thoroughly tested and validated. Statistical error has been shown to decrease with approximately the inverse first power of the sample size, as expected from the relevant kinetic theory literature. Simulations run on a Sparc 10 workstation included sample sizes up to 4 X 10⁵ molecules.

The correlation of number density and velocity components for the test case of a dilute gas in equilibrium has been examined. It has been confirmed that the number distribution of particles within each cell follows a Poisson distribution, which essentially agrees with theoretical considerations. As a further consistency check of the code, results obtained in the non-equilibrium case agree with those found in recent computational kinetic theory literature. It was found that the sampling frequency (i.e. how often one collects data to be statistically averaged) is a crucial factor in such simulations. If correlations between successive statistical samples exist, the moments of the distribution function may be significantly affected yielding misleading results.

Upon validating methods, efforts were focused on developing a 2-D cartesian code that could handle confined geometries of interest and validating it using relevant case studies. In these simulations, a strongly non-isothermal ampoule charged with Xenon was considered. Xenon is a typical background gas used in metalorganic physical

vapor transport crystal growth applications at reduced pressures. The presence of the end walls is expected to force the creep-driven gas into a circulatory motion and thus result in the formation of a vortex rotating in the counterclockwise sense. This vortical motion has been successfully captured in microscopic level simulations.

The most recent version of the DSMC code, in addition to being capable of modeling gas mixtures of arbitrary composition, incorporates appropriate end-wall boundary conditions to set up the concentration gradients necessary for concentration creep to appear. The novel computational scheme accounts for both equal and disparate mass mixtures, the latter being the more difficult since the total number of computational molecules in this case is not constant and, thus, additional bookkeeping procedures are required (also increasing by a small factor, the computational cost). Considerable effort has been invested in the disparate mass case since it is more relevant to practical applications (e.g. physical vapor transport crystal growth experiments where heavy organic substances are deposited in a light background-gas environment).

These simulations successfully capture the steady-state vortex pattern established as a result of concentration creep in the vicinity of the side walls. Computed concentration creep velocities are directed from the heavy-rich side towards the light-rich side of the ampoule, as predicted. Qualitatively, this is reminiscent of the thermal creep analog simulated early on in this grant. When compared to values predicted from one-dimensional, linearized theories, velocity scales appear to be systematically lower, mainly as a consequence of appreciable confinement effects. Such confinement effects are, of course, absent from one-dimensional theories as well as macroscopic calculations that invoke modified creep boundary conditions based on one-dimensional linearized results. This computational procedure can provide valuable insight into how to consistently extend macroscopic formulations so that rarefaction effects present can be accounted for in technological applications. Similar conclusions are drawn by comparing computed and theoretical values of the creep coefficients for both equal and disparate mass cases. In the former case, good agreement is observed, in spite of considerable differences in underlying assumptions and adversities due to the very low Mach number of the flow. Confinement effects are being fully explored and elucidated for a range of conditions and mixture compositions. For the equal mass case, a plot of the ratio of computed over theoretical creep value vs. the nominal Knudsen number with constant gradients establishes the validity of these conclusions.

In conclusion, the research activities supported by this NASA-MSAD program have led to significant developments (which have been documented in the bibliography) expected to influence the fluid physics community as well as the future of this research group.

Dimitrios Papadopoulos successfully defended his Ph.D. Dissertation entitled "Internal Flows Induced by Kinetic Boundary Layer Phenomena" which summarizes the interesting findings of a comprehensive molecular-level study of these non-continuum phenomena.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	0
PhD Students:	2	PhD Degrees:	2

TASK INITIATION: 6/94 **EXPIRATION:** 5/96

PROJECT IDENTIFICATION: 962-24-05-94

NASA CONTRACT No.: NAG3-165

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:
Journals

Papadopoulos, D.H. and Rosner, D.E., Enclosure gas flows driven by non-isothermal walls. *Physics of Fluids*, vol. 7, no. 11, pp. 2535-2537 (November, 1995).

Rosner, D.E. and Papadopoulos, D.H., Jump, creep and slip boundary conditions at non-equilibrium fluid/solid interfaces. *Ind./Eng. Chem. Research*, (September 1996).

Proceedings

Papadopoulos, D.H. and Rosner, D.E., "Fluid creep effects on near-wall solute transport for non-isothermal ampoules." *Proceedings of the Third Microgravity Fluid Physics Conference at NASA LeRC, Cleveland, Ohio, June 13-15, 1996.*

Design/Interpretation of Microgravity Experiments to Obtain Fluid/Solid Boundary Conditions in Non-Isothermal Systems

PRINCIPAL INVESTIGATOR: Prof. Daniel E. Rosner

Yale University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to design a microgravity experiment to provide unambiguous data on the appropriate thermal creep fluid/solid boundary conditions to be applied in theoretical calculations for non-isothermal systems.

Task Description:

In gas-filled ampoules that are operating under non-isothermal conditions in microgravity, it is believed that flows result in the gas due to thermal creep induced at the wall and thermal stresses in the bulk. In thermal creep, the non-isothermal walls drive a significant amount of convection and one cannot apply the traditional no-slip boundary conditions there. Following pioneering work by Maxwell, a slip boundary condition is used that is derived from kinetic theory. This boundary condition contains a slip coefficient that must be obtained experimentally. In this research the phenomenon of photophoresis, i.e., particle migration due to thermal creep which is induced by the absorption of incident radiation, is proposed to be used in a microgravity experiment to measure the slip coefficient.

Task Significance:

This research attempts to study phenomena that are not well understood. Such effects are overshadowed by convection in experiments on earth. The microgravity environment of space unmasks these phenomena and renders them amenable to experimental measurements. It is believed that these processes are important in crystal growth by physical vapor transport and chemical vapor transport (PVT and CVT) techniques.

Progress During FY 1996:

This research has been initiated in September 1996. The effort for the first year will focus on the criteria that must be met by the best microgravity experiment design in order to unambiguously interpret the photophoretic space-race of illuminated, absorbing spheres immersed in Newtonian fluids.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 9/96 EXPIRATION: 8/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-195

RESPONSIBLE CENTER: LeRC

Gas Flow from Porous Media and Microgravity Battery Spills

PRINCIPAL INVESTIGATOR: Dr. Robert T. Ruggeri

Boeing Company

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This proposal is based on the hypothesis that on-orbit spacecraft battery failures can be traced to electrolyte spills resulting from gas expanding inside the capillary pores of battery electrodes. The specific objectives of this project are as follows:

1. To determine the gas capacity of three porous metals as a function of pore volume and pore diameter.
2. To determine the system temperature and pressure effect on gas capacity.
3. To determine the effect due to the external geometry of the porous material.
4. To analytically determine the effect of gravity on electrolyte spills.

Task Description:

The objectives will be accomplished by one-g experiments and analysis. The PI will identify all critical parameters that determine a porous metal's gas capacity, then demonstrate, by measurement, the effective volume of noncondensable gas contained within the pore structure of porous metal plates as a function of the identified critical parameters. Such critical parameters are expected to be pore diameter, pore volume, sample shape, temperature, pressure and surface tension. The pore volume and the effective gas capacity of three metals will be determined in volumetric gas flow experiments. The experiments will be conducted at 25°, 45°, and 60 °C in a constant temperature chamber. Zinc, silver, and nickel are the three metals that will be investigated. The effect of pressure cycles will span a range between 14.5 psia and 2.9 psia for each temperature. One to three pressure cycles will be performed for each metal specimen at each temperature. Numerical models will be developed to study the gas capacity as a function of the pore diameter, the temperature, and the ambient pressure. The effect of gravity on these experiments will be determined analytically.

Task Significance:

Spacecraft batteries have been documented to discharge electrolyte, which causes a short circuit. The electrolyte discharging mechanism is not yet fully understood. In order to prevent mission failures in the future, critical parameters which determine a porous metal's ability to hold and discharge gas should be investigated. This will lead to design of batteries that can retain electrolyte in the microgravity environment of space and thus prevent battery failure in space missions.

Progress During FY 1996:

Two test chambers were manufactured for the experiments, however, both failed to perform satisfactorily. Test Chamber A failed catastrophically after 3-minutes at 75 psig. One lid was destroyed along with the test chamber and another lid developed a crack while being fitted with an ultra-torr fitting and is unusable until modified. Chamber B was destroyed by flying glass when chamber A exploded. Modified test plan will be provided shortly.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/94 EXPIRATION: 10/96

PROJECT IDENTIFICATION: 962-24-05-95

NASA CONTRACT NO.: NAS3-272

RESPONSIBLE CENTER: LeRC

Ground Based Studies of Thermocapillary Flows in Levitated Drop

PRINCIPAL INVESTIGATOR: Prof. Satwinder S. Sadhal

University of Southern California

CO-INVESTIGATORS:

Trinh, E.H.

Jet Propulsion Laboratory (JPL)

Task Objective:

For the measurement of the thermophysical properties of undercooled liquids, the idea of spot-heating a test sample in a levitated state is to be explored and applied to relevant materials. That is, a liquid drop levitated in an acoustic field could be heated on a small fraction of its area by a laser beam. In addition, simple filament heating will also be carried out, since this can be achieved with considerable ease. The physical interference of the filament with the fluid mechanics will of course have to be taken into consideration. By carrying out the measurements of the thermocapillary effects of such heating it is possible to derive the thermal properties of the sample. However, this can only be done with the development of a successful predictive model of the system. The effort will therefore consist of both experimental and analytical work.

1.1 Analytical Part

The purpose of the analytical part of the proposed program is to develop such a model over several phases. The major thrust at present is in ground based studies with plans for a future space experiment. In the current studies therefore, the experimentation will involve significant interference of the acoustic field. Thus, for most cases for ground based studies, the drops will be deformed to a spheroidal shape. In addition, there is general asymmetry of the flow field. While it is acknowledged that many of these complexities do not arise in low gravity, there is a great deal that can be achieved by ground based studies provided the interference by the acoustic field is fully accounted for in the analysis. For model development in the direction of a zero-g space experiment, analysis will be carried out for liquid shells and compound drops.

Under the scope of the current investigation, the analytical work will consist of several tasks that will encompass the formulation of the differential equations pertaining to levitated drops, their analytical and numerical solutions and the development of results.

1.2 Experimental Part

The experimental problem of interest in this proposal is the thermal response of a spot-heated levitated drop in a convective gas flow of varying intensity. The ultimate objective of the tasks proposed is to quantitatively determine the transient and steady-state temperature distribution on the drop surface as a function of time, sample physical properties, geometry, and of the input radiant energy. Because of the coupling of thermocapillary and thermoacoustic phenomena, the interpretation of the resulting thermal state must be carried out in conjunction with the theoretical analysis of the problem. The experimental work will thus be divided into several sub-tasks, each of which must provide data that can be directly correlated with theoretical predictions. Although the final goal will be to carry out an experiment in microgravity, this proposal will limit itself to ground-based investigations using proven experimental techniques in order to correlate with and to verify the theoretical work, as well as to develop experimental methods for a potential future microgravity investigation.

Task Description:

In the usual Earth-based environment, the convective contribution arises due to buoyancy as well as to the effects of the levitation mechanism. In this particular case, the sample may be levitated in a gaseous environment by a high intensity ultrasonic field, and the convective flow field external to the specimen is caused by acoustically-driven streaming flows in addition to the normal buoyancy-driven circulation. The heat transfer problem of determining the transient and steady-state temperature distribution at the surface of the sample will also require the solution of the flow field inside the drop driven by thermocapillary effects (and perhaps also by acoustic radiation stresses) because of the surface tension gradient introduced at the drop surface by the localized heating. Under other circumstances, the sample may be levitated in a vacuum or gaseous environment by electrostatic forces which do not generate detectable outer convective flows or droplet distortion. This approach requires, however, the permanent non-uniform charging of the drop surface; the effects of which are still unknown, but might also alter the thermally-driven capillary flows.

Under these conditions, the relevant non-dimensional parameters will thus include the Reynolds numbers of the internal thermocapillary-driven flow, of the steady outer acoustic streaming flow, and perhaps of the high frequency acoustic particle motion. The Bond number will be of relevance in order to distinguish between low gravity and Earth-based conditions. The Nusselt, Grashof and Marangoni numbers will also play a primary role. Because we shall be restricted to rather moderate temperature and to conditions far enough from the boiling point of the liquids investigated, mass transfer processes will not be taken into consideration in this case.

Task Significance:

The proposed research will provide fundamental understanding of the Marangoni flows associated with localized heating of drops and bubbles. For ground based studies where there is interference from the acoustic field, a sound numerical model will provide significant new information about the behavior of these complex systems. The new work on compound drops will play a fundamental role for a zero-g space experiment. Most importantly, the model development along with the experimental studies will represent fundamental groundwork for the measurement of thermophysical properties of undercooled liquids.

Progress During FY 1996:

Experimental Results

Studies of Acoustic Streaming

Flow visualization studies of the external forced convective fields generated by the high intensity ultrasound used to levitate millimeter-size droplets under the full effect the Earth gravitational field have been previously reported. The increase in the heat and mass transfer coefficients between a levitated liquid drop and the surrounding gas has been quantitatively evaluated. In addition to affecting the transport process, external flows also induce low velocity internal flows due to entrainment. Arising from the time-varying acoustic motion and from the steady streaming flow component, this entrained flow field is weak for the case of a liquid drop levitated in a gas. It can be substantial, however, for a drop levitated in an immiscible liquid host has been used to record the motion of fluorescent tracer particles suspended in the drop liquid. Polystyrene particles of Florida Yellow G from Bangs Laboratories having 0.405 microns in average diameter have been visualized using an Argon Ion (488 nm) laser sheet with variable orientation (the sheet thickness is about 200-300 microns). The scattered light is gathered along two orthogonal views using holographic notch filters to block the elastically scattered light from the drop surface. The liquid used was an aqueous mixture of glycerin and silicone oil (Polydimethylsiloxanes) and a focused CO_2 laser was used to spot heat the levitated drop. The results show that although it was possible to accurately measure the internal flows of isothermal drops, the combination of Earth-based levitation and spot heating induces an uncontrolled torque which drives a random rotational motion of the drops. The digital image processing required in the deconvolution of this rotational motion in order to extract the thermocapillary and buoyancy-driven flows requires substantial computational power, and will be pursued by this experimental effort. In general, all the recorded flow fields have lacked axial symmetry although both the levitation apparatus and the heating direction are axially symmetrical. Control of drop evaporation has been implemented by maintaining the drop environment at a high humidity, and the Marangoni convection contribution due to evaporation can thus be neglected. Ongoing and future studies will include the measurement of flows within significantly flattened drops to constrain the flows in a two dimensional plane, the implementation of total electrostatic levitation of charged droplets, and an automated digital data reduction and analysis.

Glovebox Low-Gravity Demonstration

A Glovebox flight investigation scheduled for the MSL-1 in April 1997 has been initiated to assess the capability for ultrasonic positioning in microgravity for drop internal flow measurement. A compact ultrasonic positioner has been designed and integrated with laser diode illumination in order to experimentally demonstrate the rotation control of freely suspended drops in low gravity and to obtain preliminary flow field measurements for sting-heated droplets. A laboratory breadboard is already available, and the flight unit is currently nearing design completion.

Analytical Results

Spherical Particle at the Velocity Node of a Standing Wave

Analytical studies have conducted for a spherical particle suspended at the velocity node. The complete singular perturbation analysis of the exterior acoustic flow has been carried out for small values of the Reynolds number, the streaming Reynolds number at high frequency. As expected there is a net steady-state flow field. Some interesting

flow patterns have been predicted. While there is a thin layer on the surface of the particle, as in the case a particle at the velocity antinode, the streamlines are not closed. The reverse flows within the layer exist only for a belt-shaped region about the equator. Specifically, for angular positions between 55 degrees and 125 degrees with the polar axis, the thin layer of reverse flows is found. These values correspond to $\cos 2 \{\theta\} = -1/3$. Outside this range, around the polar regions, the streamlines merge with the exterior flow. Mathematically, this behavior results because the Stokes-layer solution consists of two components corresponding to the first and the third spherical harmonics. These solutions add up with two guaranteed zeros in the radial direction only for a limited region over the sphere as discussed.

Oblate Spheroid at the Velocity Antinode

The leading-order solution for a deformed particle at the velocity antinode has been found. Presently, there are some analytical difficulties with obtaining higher-order solutions. The steady components of the flow field have therefore not been found yet. If further attempts do not yield a valid solution, numerical solutions will be sought.

Internal Circulation in a Drop in an Acoustic Field

The investigation of the internal flow in a drop at the antinode of a standing wave has been carried out by singular perturbation approach. At the fluid-fluid interface, the stress and velocity continuity condition are applied. It is observed that the strength of this internal flow is extremely weak. The reason for such weak flow is mainly the recirculating Stokes layer which is very thin. Since there are opposing velocities within it, a very large shear stress is required to sustain its motion. The system cannot afford such a large shear stress at the interface and the result is weak internal circulation. The large drop viscosity as compared with the gas also has a role in weakening this circulation. While experimental studies also show a weak internal circulation, the magnitude has not yet been verified to be in agreement with the extremely low predictions. One possible explanation is that with the experiments, the recirculating Stokes layer may only partially cover the drop as predicted for particle at the velocity node, leaving the possibility of significant vorticity transfer across the interface.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 1/93 EXPIRATION: 12/96

PROJECT IDENTIFICATION: 962-24-07-19

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Books

Sadhal, S.S., Gopinath, A., Oosthuisen, P.H., and Hashemi, A. "Proc. 30th National Heat Transfer Conference - 1995, Vol. 3, "Heat Transfer in Microgravity Systems." Edited by: HTD-Vol. 305, ISBN 0-7918-1704-0 ASME, New York, Vol.3, pp 193, 1995.

Presentations

Sadhal, S.S. "Acoustically levitated drops." Invited lecture, Gotas, burbuja y peliculas (Drops, bubbles & films), Escuela de Fisico-Quimica de Fluidos, Universidad Internacional Menendez Pelayo, Santander, Spain, September 9-13, 1996.

Zhao, H., Sadhal, S.S., and Trinh, E.H. "Singular perturbation analysis of an acoustically levitated sphere." Western States Section of the Combustion Institute, Fall 1996 Meeting, Los Angeles, October 1996, Paper No. 96F-126.

Ground Based Studies of Internal Flows in Levitated Laser-Heated Drops

PRINCIPAL INVESTIGATOR: Prof. Satwindar S. Sadhal

University of Southern California

CO-INVESTIGATORS:

Trinh, E.

Jet Propulsion Laboratory (JPL)

Task Objective:

The objective of this research is to determine the thermophysical properties of liquids in their undercooled states. These properties will be inferred from measurements of the characteristics of thermocapillary flow induced by spot heating a levitated sample.

Task Description:

The objectives will be accomplished by theoretical modeling and experimental observations. The levitation of the liquid sample is by acoustic and electrostatic means. With both types of levitation techniques, additional flows are expected in the sample that must be accounted for. The thrust of the theoretical effort is to predict the internal circulation in spot heated drops, understand the extent to which interference is caused by the levitation forces and calculate the deformations of the drop. The goal of the experimental program is to measure the strength of the internal circulation and the temperature distribution on the drop surface as a function of time, sample physical properties, geometry and the heat flux to which the sample is subjected. Because of the coupling of thermocapillary flow with acoustic and electrostatic levitation forces, the interpretation of the observed internal flows and thermal state must be carried out in conjunction with the theoretical analysis of the problem.

Task Significance:

In levitated liquid samples on the earth as well as under conditions of microgravity in actual space-flight, materials can be processed without permitting them to be in contact with a container. This permits the liquid to be undercooled deeply below its normal freezing temperature and is believed to lead to the development of new materials such as certain types of crystals with high homogeneity and composites with fine and even distribution of the dispersed phase.

Progress During FY 1996:

This research was initiated in June 1996. The study for the first year will (i) lay the theoretical framework for subsequent analytical and numerical investigations (ii) measure the background flow fields in unheated and uncharged drops due to acoustic and electrostatic levitation forces.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-184

RESPONSIBLE CENTER: LeRC

Effects of Gravity and Shear on the Dynamics and Stability of Particulate and Multiphase Flows

PRINCIPAL INVESTIGATOR: Prof. Ashok S. Sangani

Syracuse University

CO-INVESTIGATORS:

Koch, D.L.

Cornell University

Louge, M.

Cornell University

Task Objective:

The main objectives of this project are to understand the differing particulate and multiphase flow behaviors that will occur in space and in Earth's gravity. More specifically, the project is concerned with understanding the effects of shear and gravity on two relatively ideal suspensions with significant inertial effects. The first is a gas-solid at small Reynolds Numbers and finite Stokes numbers. In this type of suspensions, the inertia of the particulate phase is significant while the hydrodynamic interactions are dominated by viscous forces in the suspending fluid. The other is a bubble suspension at small Weber and large Reynolds numbers. The hydrodynamic interactions in such suspensions are dominated by the inertial effects in the suspending fluid, but these inertial interactions can be described using potential flow theory. Our main objective is to examine the effects of shear and gravity on the average properties and stability of these two suspensions.

Task Description:

Complementary theoretical, simulation and experimental approaches to achieve the aforementioned task objective. The study will consider two types of inertial suspensions that are amenable to detailed theoretical studies. The first type is a solid-gas suspension, in which the inertia of the particle and the gas viscosity are more important than the gas phase inertia. The second type is a suspension of bubbles with high Reynolds number indicating inviscid flow, but with small Weber number indicating that their deformation is small. Theoretical development of sheared particulate and bubbly liquids will make use of concepts borrowed from the kinetic theory which has been successfully applied to granular flows. The kinetic theory will be complemented by a numerical simulation of the solid-gas and gas-liquid suspensions. These simulations include detailed calculation of the hydrodynamic interactions among the particles in both microgravity and Earth gravity conditions. To validate the equation of motion of the suspension systems, experimental measurements of suspension properties in simple basic flow situations are necessary. The initial Earth-based experiment will involve a sheared fluidized bed by using capacitance probes to measure the volume fraction as a function of time, the shear rate required to overcome the gravitational instability. The knowledge gained from the theoretical, simulation, and experimental work will set the necessary background to propose low gravity experiments.

Task Significance:

Our current understanding of suspensions in which the inertial effects are significant is very limited. The two suspensions studied under this project are amenable to detailed numerical and theoretical analyses and therefore serve as ideal suspensions for understanding the effects of inertia. Gas-solid suspensions and bubbly liquids are also encountered in many industrial processes and therefore it is of great interest to determine the average equations for their flow and the conditions under which stable flows of these suspensions can be sustained.

Bubbly liquids are encountered in many heat and mass transfer operations such as the reboiler of a distillation column or heat exchangers in chemical and nuclear plants. An accurate description of the flow and heat transfer characteristics of bubbly liquids is very important in designing safe, efficient chemical and nuclear plants. Sheared and fluidized particulate flows are important in technologies for clean utilization of coal.

Progress During FY 1996:

We have completed detailed theoretical and numerical studies of sheared gas solid and bubbly suspensions¹⁻³. A kinetic theory was developed in Ref. 1, 2 for the simple shear flows of gas-solid suspensions to predict the particulate-phase stress in terms of volume fraction of solids, Stokes number, and the coefficient of restitution characterizing the inelastic collisions among the particles. The predictions of the theory were shown to be in excellent agreement with the results of numerical simulations.

In Ref. 3, we developed a similar kinetic theory for bubbly suspensions and it was shown that the predictions of this theory are also in excellent agreement with the results of numerical simulations of sheared bubbly suspensions for a wide range of bubble volume fraction and Reynolds numbers.

In addition, we have performed simulations of bidisperse gas-solid suspensions in the presence of gravity and determined the conditions under which the uniform state of the suspension becomes unstable. The instability was shown to lead to partial segregation of the two solid species. This work will be presented at the American Physical Society meeting this fall.

We have designed and built a couette cell to explore the effects of shear flow on fluidization. Kinetic theories of the type mentioned above predict that the shearing motion will increase the particulate-phase pressure and stabilize the homogeneous state of the fluidized bed. Our preliminary observations of the sheared fluidized bed confirm that shearing inhibits bubbling.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	.5	MS Degrees:	1
PhD Students:	1	PhD Degrees:	0

TASK INITIATION: 5/94 **EXPIRATION:** 5/96**PROJECT IDENTIFICATION:** 962-24-05-96**NASA CONTRACT NO.:** NAG3-163**RESPONSIBLE CENTER:** LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Kang, S.-Y., Sangani, A. S., Tsao, H.-K., and Koch, D.L., Rheology of dense bubble suspensions. *Phys. Fluids*, (1996).

Sangani, A.S., Mo G., Tsao, H.-K., and Koch, D.L., Simple shear flows of gas-solid suspensions at finite stokes numbers. *J. Fluid Mech.*, 313, pp. 309-341 (1996).

Tsao, H.-K. and Koch, D.L., Rapidly sheared, dilute gas-solid suspensions. *J. Fluid Mech.*, 296, pp. 211-245 (October 1995).

Presentations

Mo, G., Sangani, A.S., Tsao, H.-K., and Koch, D.L., "Simple shear flows of dense gas-solid suspensions at finite Stokes numbers." Annual Meeting of American Institute of Chemical Engineers, Miami, FL., October 1995.

Sangani, A.S., and Koch, D.L., "Rapidly sheared bubble suspensions." Third Microgravity Fluid Physics Conference, NASA Lewis Research Center, Cleveland, OH, June, 1996.

Valiveti, P. and Koch, D.L., "Instabilities of bidisperse sedimenting gas-solid suspensions." American Physical Society Division of Fluid Dynamics Meeting, Syracuse, NY, 1996.

Dielectric and Electrohydrodynamic Properties of Suspensions

PRINCIPAL INVESTIGATOR: Dr. Dudley A. Saville

Princeton University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This investigation focuses on understanding those electrokinetic properties of particulate suspensions related to the so-called "electrohydrodynamic effect," specifically, the dielectric constant and electrical conductivity. These properties are of crucial importance in defining the behavior of samples in various electrokinetic separation processes. The work involves two research tasks:

1. Measurements of the electrokinetic properties of a series of suspensions with particle volume fractions between 1% and 20% by volume.
2. Development of a theory for the dielectric constant and conductivity of suspensions which encompasses the measured behavior.

Task Description:

Experimental work: We have been attempting to prepare model particles which conform to the classical theory. Previous research showed that with some particles annealing at 120 °C (above the glass transition temperature) smoothed the particle surface so suspensions behaved according to the classical theory. Attempts to prepare such particles using both anionic and amphoteric latexes purchased from the Interfacial Dynamics Corporation met with limited success. The reasons for this behavior are not at all clear. Accordingly, we have been working to adsorb polymer on latex particles to increase their dipole moment. Suspensions prepared with these particles will have large dielectric constants which can be controlled by the amount and size of the adsorbed polymer.

Theoretical work: We continue to work on theoretical models of the electrohydrodynamic effect and on models of the electrokinetic behavior of dispersions. The purpose of these efforts is to provide the requisite theory to interpret our results.

Task Significance:

This research is intended to develop an understanding of one of the major obstacles to the effective separation of particles by electrokinetic methods. Moreover, we have uncovered ways of adapting our techniques to providing an understanding of the behavior of particles in nonaqueous systems. Thus, in addition to its applications to separations, our work should be useful in materials processing.

Progress During FY 1996:

During the past year three activities were pursued: the behavior of fuzzy particles, improving our dielectric spectrometer, and work on non-aqueous systems. The Ph.D. student has finished her experimental work on fuzzy particles and is completing a Ph.D. thesis. A new spectrometer was assembled and tested to verify its performance. Finally, we completed work on non-aqueous systems, showing they are subject to the same "electrohydrodynamic effects" as are aqueous systems. This is the final year of the task and a proposal was submitted in response to a new NRA.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 6/91 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-24-08-08

NASA CONTRACT NO.: NAG8-878

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Barchini, R., and Saville, D.A. Dielectric Response Measurements on Concentrated Dispersions. *J. of Colloid & Interface Science*, vol. 176, 86-91 (1995).

Barchini, R., and Saville, D.A. Electrokinetic Properties Of Surfactant Stabilized Emulsion Droplets. *Langmuir*, vol. 12, 1442-1445 (1996).

Gittings, M.R., and Saville, D.A. Electrophoretic Mobility and Dielectric Response Measurements on Electrokinetically Ideal Polystyrene Latex Particles. *Langmuir*, 11798-11800 (1995).

Trau, M., Sankaran, D.A., and Aksay, I.A. Field-Induced Layering of Colloidal Crystals. *Science*, vol. 272, 706-709 (1996).

Trau, M., Sankaran, S., Saville, D.A., and Aksay, I.A. Electric Field-Induced Pattern Formation In Colloidal Dispersions. *Nature*, vol. 374, 437-439 (1995).

Trau, M., Sankaran, S., Saville, D.A., and Aksay, I.A. Pattern Formation in Non-Aqueous Colloidal Dispersions via Electrohydrodynamic Flow. *Langmuir*, 114665-114672 (1995).

Presentations

Saville, D.A., Trau, M., and Aksay, I.A. "Electrohydrodynamics of aqueous colloidal dispersions: particle deposition and assembly on surfaces." American Institute of Chemical Engineers, 1995 Annual Meeting, Miami, Florida, November 1995.

Saville, D.A., Trau, M., and Aksay, I.A. "Field-induced two and three-dimensional colloidal crystals." 1995 Materials Research Society Meeting, Boston, Massachusetts, November 1995.

Terrestrial Experiments on G-jitter Effects on Transport and Pattern Formation

PRINCIPAL INVESTIGATOR: Dr. Michael F. Schatz

Georgia Institute of Technology

CO-INVESTIGATORS:

Swinney, H.L.

University of Texas, Austin

Task Objective:

This ground-based experimental program will investigate the effects of time-dependent acceleration (g-jitter) on fluid systems with density variations. Results from this work will be compared to theory and to experiments aboard spacecraft.

Task Description:

A unique vibration test facility is being developed to expose simple fluid experiments to a wide range of acceleration conditions. The fluid experiments include studies of particle motion, thermal convection, and mass diffusion; the physical properties of the experiments will be adjusted to provide dynamic similarity with microgravity experiments. The experiments will be subjected to time-dependent accelerations whose root-mean-square far exceeds the mean, as is typical in space. The computer-controlled test facility will provide acceleration profiles that emulate those measured aboard spacecraft.

Task Significance:

All microgravity experiments experience unavoidable time-dependent accelerations (g-jitter) arising from spacecraft operations (e.g., thruster firings). Although it is known that g-jitter can influence the outcome of space experiments, the effects on g-jitter are not adequately understood. This ground-based work systematically probes the primary ways g-jitter can influence fluid experiments. Direct comparison of data from the experiments with theoretical and numerical models of g-jitter effects should lead to the development of better models for g-jitter, which should enhance the chances of success for future space experiments.

Progress During FY 1996:

Work on this task was initiated with the start of funding in June 1996. Progress to date (4 August 1996):

- Purchase of vibration test facility has been initiated. A high-performance hydraulic test system is being custom designed to provide a wide range of computer-controlled time-dependent accelerations for the experiments.
- Experiment construction has begun. A Rayleigh-Bénard convection cell has been designed and is being fabricated. The Rayleigh-Bénard experiment with time-dependent acceleration is expected to yield new insight into the physics of pattern formation and will serve as a good test problem to validate the operation of the new vibration test facility.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 0

TASK INITIATION: 6/96 EXPIRATION: 4/00

PROJECT IDENTIFICATION: 963-24-00

NASA CONTRACT NO.: NAG3-187

RESPONSIBLE CENTER: LeRC

Free-Surface and Contact-Line Motion of Liquids in a Microgravity Environment

PRINCIPAL INVESTIGATOR: Dr. Leonard W. Schwartz

University of Delaware

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The purpose of this research is to further apply and/or develop a model for the slow spreading of liquids on a variety of surfaces (mixed wettable, macroscopically roughened, etc.) and perform three-dimensional unsteady computer simulations of the flow.

Task Description:

The investigation incorporates analysis, numerics and experiment, and will cover a range of solid substrate geometry, wettability, and roughness.

Task Significance:

Though insights gained from such investigation are of intrinsic scientific value and are very applicable to many current Earth-based applications, such flows are also of key concern to many if not all fluids handling operations in space.

Progress During FY 1996:

We have formulated a model for the slow spreading of liquid drops on a mixed wettable surface and performed three-dimensional unsteady computer simulation of this process. We find that substrate energetics, as represented by the static contact angles on the wettability pattern, provides the driving force for the motion. The simulation results exhibit a number of features including characteristic 'jerky' motions and drop breakup. Quite recently, experimental observations performed by R. R. Eley (ICI/Glidden Paints) have confirmed specific predictions of the model. This problem is relevant to the control of liquid masses in microgravity when contact line pinning and dissipation is used as a control mechanism.

A related problem involves the use of surface roughness rather than wettability variation. We are performing three-dimensional unsteady calculations of the forced motion of thin liquid films over periodic and disordered patterns of surface roughness. It is of interest to determine the similarities and the differences between these two methods of surface treatment. To the extent that confining surfaces are not planar, motion of liquid films on curved surfaces is also of interest. We have recently completed a study concerning simulations of coating layer evolution and drop formation on horizontal cylinders.

The above work employs the small-slope, slow-motion form of the governing equations and, as such, is relevant only to a portion of the flow domain when liquid masses are in motion. The 'outer' problem, away from the walls is being treated as an unsteady potential flow with moving boundaries and capillarity. The solution is being obtained using a boundary integral or 'panel' method. We have successfully simulated unsteady motion of two-dimensional isolated liquid masses and will shortly treat the axisymmetric case. When the initial surface differs only slightly from a circle, the subsequent periodic motion agrees with the classical linear solution of Rayleigh.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 7/96 EXPIRATION: 7/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-192

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Schwartz, L.W., Simulation of droplet motion on heterogeneous surfaces. *Physics of Fluids*, (1996).

Weidner, Schwartz, L. and Eres, Simulation of coating layer evolution and drop formation on horizontal cylinders. *J. Colloid & Int. Sci.*, (1996).

Drop Breakup in Flow through Fixed Beds as Model Stochastic Strong Flows

PRINCIPAL INVESTIGATOR: Dr. Eric S. Shaqfeh

Stanford University

Co-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Our objective in the research as described in our proposal is to examine, both theoretically and experimentally, the deformation and breakup of drops in the flow through fixed particle beds. In particular the focus will be on fixed fiber beds at low to moderate volume fraction with the immediate application to the emulsification of liquids via the use of fibrous filters. However the research also has application to the oxygenation of plants in artificial soils and we intend this to be a future focus. The broader aims of the research are to examine drop breakup in Lagrangian unsteady and disordered flow fields of which fixed bed flow is an example. In this context, the application is to examine how drops breakup in random flow fields such as those experienced under g jitter conditions.

Task Description:

The two principal parts to the research are (a) the development of large scale computer simulations of drop deformation and breakup in rapidly Lagrangian time varying flows and (b) a complete set of experiments which alleviate gravitational effects yet allow for the determination of drop breakup conditions in the flow through moderately dilute fixed fiber beds.

Task Significance:

The tremendous fundamental significance of this work lies in the potential for understanding drop breakup in disordered and time varying flows. Work on drop breakup has focused almost exclusively on breakup in steady flows, and the work which exists regarding time varying flows has not centered on disordered or random flows. Disordered flows, (e.g. turbulent flows, flow through networks, flow with suspended particles, etc.) are omnipresent and of great practical importance. There is every reason to believe from a host of other work in flow through fixed beds that their disordered nature can create qualitatively different effects (e.g. efficient breakup), while it is just this disorder which can allow modern statistical mechanical techniques to be applied toward their understanding. Moreover, there are immediate practical applications to this study including the understanding of the use of fibrous filters as emulsifiers, plus the potential for a different approach to the examination of drop breakup in soils and more complicated porous media.

Progress During FY 1996:

We have completed the development of a large scale simulator of drop breakup in the flow through dilute fixed beds. The simulator rests on the relationship between flow through dilute fixed media and a certain class of anisotropic Gaussian flow fields, as originally derived by Shaqfeh and Koch (1992). Thus we create an appropriate realization of the anisotropic Gaussian flow field using spectral techniques originally applied to the simulation of turbulent flows (Mosler and Shaqfeh, 1996; Kraichnan, 1970). As an initial model for the drop we use the first, second and third order small deformation theories developed by Barthes Biesel and Acrivos (1973). We then follow the deformation of these model drops as they flow through a large number of realizations of the flow, and collect all the statistical information necessary to describe the deformation and breakup process. The important parameters are the three deformation parameters (in the three orthogonal planes), and the principal directions of the deformation, both as a function of the pore-size or fluctuation Capillary number. Note in this context that the correlation length of the fluctuations is directly related to the pore size (and therefore the solids volume fraction) in the model porous media, and thus the volume fraction is a final important parameter. Our findings as delineated in the figures are as follows:

1. Large deformation and breakup of drops occurs in the flow as predicted by the second and third order small deformation models. Note this is very similar to the predictions of these models in steady, classical strong flows. However, the mean deformation of the drops remains small, but breakup (defined as unbound deformation parameters) occurs from the large deformation tails of the distribution. The distribution itself is rather broad for Capillary numbers in excess of 0.05.

2. The critical Capillary number for breakup events is approximately 0.15 which is again very comparable to critical conditions for classical, steady strong flows. However, the mean deformation of the drops at this value is still very small, breakup events are focused in the tails of the distribution.

3. Beyond the critical Capillary number the rates of drop breakup increase strongly, and ultimately the breakup rate (measured as a fraction of the existing population of drops) is linear in the Capillary number. A simple description of this has been developed based on the fact that the drop deformation is approximately quadratic in the local rate of deformation tensor. However the sampling time decrease linearly as the Capillary number increases. Thus, since breakup is correlated with a critical extent of deformation, the rate of exceeding that critical deformation is approximately linear in Capillary number.

4. The breakup events are, for the most part, shear breakup events rather than extensional flow breakup. After careful examination, the angle of the largest drop extension is actually very close to 45 deg from the direction of the mean flow. Thus, even though the average flow is axisymmetric about the mean flow direction, stretch is primarily occurring along the 45 degree line - just as in a shear flow.

We are beginning to develop and are looking forward to an experimental examination of drop breakup in the flow through dilute fixed media.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/96 **EXPIRATION:** 5/97

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-184

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Mosler, A.B. and Shaqfeh, E.S.G., The conformation of model polymers in stochastic flow fields: Flow through fixed beds. Phys. Fluids, (June 1996).

Electrohydrodynamic Pool Boiling in Reduced Gravity

PRINCIPAL INVESTIGATOR: Prof. Benjamin D. Shaw

University of California, Davis

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

To investigate the effects of electric fields on reduced-gravity pool boiling. The electric fields are expected to significantly and controllably increase reduced-gravity nucleate boiling rates and maximum heat fluxes. The presence of an electric field will result in the production of smaller bubbles in reduced gravity and the average speed of bubble production will be increased.

Task Description:

A apparatus to study boiling has been constructed for use at the NASA Lewis 2.2 Second Drop Tower. This apparatus will consist of a pool boiling test chamber and associated instrumentation mounted on a NASA drop frame. Boiling will occur on an electrically-heated platinum wire subjected to a nonuniform external DC electric field. Boiling experiments with FC-72 or FC-87, (for which $tc \gg tb$) or water (for which $tc \ll tb$) will be performed in both 1-g and μg . Data will be gathered on applied electric fields and wire heat fluxes and temperatures. High-speed motion picture photography will provide visual records of boiling phenomena.

Task Significance:

Anyone who has ever boiled water on a stove is familiar with nucleate pool boiling. Even though it is an everyday event, scientists do not understand precisely how it works, because the Earth's gravity influences how bubbles form and grow in boiling liquids.

NASA is interested in the results from this experiment, because boiling liquids generate bubbles which are very efficient at transferring large amounts of heat. Finding new ways to dissipate heat from the space shuttle or future manned space platforms will be vital to the success of long-term missions.

The potential benefits closer to home, including more effective air conditioning and refrigeration systems, and improvements in power plants that could reduce the cost of generating electricity.

Progress During FY 1996:

The initial efforts of the past year focused upon designing an experiment to study the effects of applied electric fields on reduced-gravity pool boiling occurring with thin platinum wires heated in a host fluid. Calculations were performed to identify the experimental conditions (e.g., wire diameters, host fluids, etc.) that would be most likely to yield the best experimental data. It was decided that three fluids would be used: water, and the chlorine-free refrigerant (and environmentally friendly) FC-87 or FC-72. A prototype boiling chamber was subsequently built and tested with water. This chamber helped us to determine the best way to support the wire and allowed us to test critical electronic components (e.g., a programmable microcontroller and programmable power supply) needed for the boiling experiments. In addition, different lighting arrangements for the experiments were evaluated with this prototype chamber, and a suitable lighting scheme was selected. All of the components and materials needed to construct the apparatus have now been designed and/or acquired (e.g., high-voltage power supplies, the platinum wire power supply, batteries, battery boxes, the drop frame, the boiling chamber, control electronics, boiling chamber insulation, boiling chamber heaters (cartridge and tape), a special flexible bladder to allow for volume expansion without significantly raising the chamber pressure, etc.). Construction of the apparatus is now completed and normal gravity experiments are underway. Reduced-gravity experiments (50 to 100 drops are planned) will be performed at the NASA Lewis Research Center in the fall of 1996.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 1

PhD Students: 0

TASK INITIATION: 6/94 **EXPIRATION:** 12/96**PROJECT IDENTIFICATION:** 962-24-05-97**NASA CONTRACT No.:** NCC3-353**RESPONSIBLE CENTER:** LeRC

Transport Processes Research

PRINCIPAL INVESTIGATOR: Dr. Bhim S. Singh

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this task is to promote, foster, and enhance the quality and breadth of microgravity research conducted in the discipline of fluid physics by advancing the understanding of thermal and mass transport processes when buoyancy-driven convection is reduced or eliminated.

Task Description:

The approach to achieving the task objective is to provide LeRC in-house support to assist sponsored principal investigators in the conduct of their research (particularly when that research can benefit from unique expertise or facilities at LeRC), while guiding and assisting in the definition of flight experiments.

Task Significance:

This task will assist in program planning and outreach programs in the external community, and it will conduct in-house research to advance the understanding of transport and interfacial phenomena through exploitation of the microgravity environment.

Progress During FY 1996:Ground-Based Facility Support to Principal Investigators:

Support was provided to continuing the study of absolute instability of liquid jet in microgravity using Lewis' 2.2 Second Drop Tower. Prof. Lin (Clarkson University) and his students conducted 96 drops using their specially designed Drop Tower rig with the help of Lewis personnel. They also utilized Lewis developed TRACKER software to analyze the results from their Drop Tower tests. We provided support to Prof. Ronney (University of Southern California) on studies of Radiation-Driven fluid flow and heat transport. Prof. Ronney's student conducted successful drops in the Lewis' 2.2 Second Drop Tower. Assistance was also provided to Prof. Shaw (University of California, Davis) in his study of Electrohydrodynamic Pool Boiling in Reduced Gravity for his 2.2 Second Drop Tower tests. We also assisted a number of PIs in planning and conducting tests on Lewis' Reduced-Gravity Aircraft (DC-9). Prof. Saville (Princeton) conducted tests to evaluate design concepts and operational strategies for his flight experiment entitled "Studies in Electrohydrodynamics." Prof. Carey (University of California, Santa Barbara) conducted pioneering experiments on Marangoni Effects in Boiling of Binary Fluid Mixtures under Microgravity. Dr. Abdollahian (S. Levy, Inc.) conducted studies of two-phase and heat transfer in reduced gravity. In all of these Lewis scientists not only provided assistance in planning and advising the PIs but actively participated in conducting the tests onboard the Aircraft. Lewis also provided high speed video imaging system and photography assistance.

Marangoni-Benard Instability (MBI):

The 3-D numerical simulation of the Marangoni-Benard Instability has been completed with the critical Marangoni number and the convection pattern at the onset of M-B-I predicted for 4 different aspect ratios. The numerical results agreed very well with existing analytical and experimental data. More in-depth studies will require significant resources and is not planned for the near future. Dr. J.C. Duh has continued working with Prof. Alex Oron, who visited LeRC in August, on using combined analytical/numerical analysis to study thin liquid film subject to a vertical temperature gradient. This study includes the Marangoni effects, the surface deformation, and the disjoining pressure in the model. Both onset of the instability and the break-up of the thin film are investigated. The results will be presented in a future microgravity fluids conference.

Thermocapillary Migration of Bubbles and Drops:

Dr. Balasubramaniam has worked on the following theoretical problems in this area: i) Analysis of the motion of drops with strong internal circulation. The analysis has almost been completed. It has revealed that the transport inside the drop gives rise to a regime of migration that has not been reported in the literature. As a consequence, the

velocity scale for the drop motion is quite different from the previously published results. It has also been shown that in the gas bubble limit, known results are recovered. ii) Analysis of the interaction of two bubbles when the Marangoni number is large. Here the goal is to capture the effect of the thermal wake of the leading bubble on the motion of trailing bubble. A model is being formulated that is capable of predicting these effects.

Two-Phase Flow in Microgravity Environment:

Dr. S. Jayawardena (NRC) conducted two sets of reduced gravity two-phase flow experiments at a pipe junction using the Lewis' DC-9 aircraft, in October and December 1995. These tests provide observations and data on the behavior of such flows at three different liquid flow rates and about five different gas flow rates, using fluids with different physical properties. The collected data was analyzed and two papers were presented at national meetings.

He also continued to refine the two-phase flow diagnostics flow loop, which was used for calibration of the sensors used in the above tests. Two other researchers, Sal Paise and Ed Keshock are currently using that facility to conduct experiments. A proposal submitted to the 1994 NRA by Jayawardena with Prof. Balakotaiah (PI) of the University of Houston has been selected as a flight definition and he is presently working at University of Houston.

Capillary Driven Flows:

The general problem of capillary flow in containers with interior corners and several flows in which the moving contact line plays a dominating role have been addressed both experimentally and analytically. The experimental portion of the work required the collection of a large data set incorporating both drop tower and DC-9 aircraft testing. Specific data regarding flow rate measurements of spreading drops and the inhibition of fluid in square, rectangular, and triangular cross-sectioned cylinders were collected. The problem of spontaneous capillary flows due to variable surface wetting properties was also investigated using both laboratory and drop tower tests.

Parallel theoretical studies were completed and a family of similarity solutions was found for the general problem of capillary driven flow in interior corners. The important features of the flow could be expressed in explicit forms and very useful information concerning time response, spreading rates, and stability of the flow is now discernible. Comparison with the data shows good quantitative agreement. These results add significantly to our ability to design systems for use in space. For example, the optimum groove geometry can be computed for a given application (heat pipe condensate return, condenser geometry, ullage positioning in liquid tanks, etc.), or the optimum fill rate of a complex container in low-gravity can be estimated.

This work has been in part conducted to support the flight experiments ICE-Mir (Interface Configuration Experiment, PI: P. Concus) which flew on USML-2, Nov. 1995, DYLCO (Dynamics of Liquids in Edges and Corners, PI: D. Langbein) which flew on the MAXUS sounding rocket, Jan. 1996, and ALB (Angular Liquid Bridge experiment, PI: P. Concus) a Mir Glovebox experiment to fly Jan 1997.

Thermocapillary Flow in an Evaporating Layer:

Dr. Zhang (NRC) devised and conducted a series of experiments to investigate the thermocapillary flows in an evaporating liquid layer. Benard cell formation was observed and recorded when liquid layers evaporate in open air at room temperature with and without cooling from below. Flow patterns and wavelengths in evaporating layers were recorded and analyzed. It was concluded that the traditional theory of Marangoni - Benard instability may not be applicable to the case of evaporating layers. Dr. Chai served as Dr. Zhang's research advisor.

Others:

The gravity modulated Benard problem was investigated. The thin unbounded fluid layer with free and fixed surfaces was considered. Surface tension variation at the free surface was also included. Finger shaped instabilities were observed in (g , $1/W$) space for both the modulated Marangoni problem and modulated Rayleigh problem. In the case of the modulated Marangoni problem, the fingers were much more elongated. The gravity modulated doubly diffusive Marangoni problem has briefly been investigated as well. A resonance behavior was observed when modulation was applied in the presence of overstability (oscillatory instability). The systems are still far more sensitive to lateral free surface disturbances.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 4 BS Degrees: 4
MS Students: 0 MS Degrees: 0
PhD Students: 0 PhD Degrees: 0

TASK INITIATION: 1/94 EXPIRATION: 1/97

PROJECT IDENTIFICATION: 962-24-05-01

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Balasubramaniam, R. and Subramanian, R.S., Thermocapillary bubble migration - thermal boundary layers for large Marangoni numbers. *Int. J. Multiphase Flow*, vol. 22, no. 3, pp 593 - 612 (1996).

Oron, A., Deissler, R., and Duh, J.C., Marangoni convection in a layer with two free surfaces. *European Journal of Mechanics, B/Fluids*, vol.6, pp. 737-760 (November 1995)

Weislogel, M.M., Capillary flow in an interior corner, UMI dissertation information service. Ph.D thesis, Northwestern University, Evanston, IL, (1996).

NASA Tech Briefs

Weislogel, M.M., Capillary flow in an interior corner, UMI dissertation information service. Ph.D thesis, Northwestern University, Evanston, IL. NASA Tech Brief, (1996).

Proceedings

Balakotaiah, V. and Jayawardena, S. S., "Stability of wavy films in gas-liquid two-phase flow at normal and microgravity conditions." *Proceedings of the 3rd Microgravity Fluid Physics Conference*, NASA CP-3338, 1996.

Jayawardena, S.S., "Reduced gravity two-phase flow at a tee-junction." *Proceedings of the 31st National Heat Transfer conference*, Houston, TX, August 1996.

Presentations

Duh, J.C. and S. Yu and B. Jiang, "Three-dimensional simulations of Marangoni-Benard convection by the least-square finite element method." presented at 1996 AIAA Symposium on Microgravity Science, 1996.

Jayawardena, S.S., "Two-phase flow at a pipe junction - slug flow." *AICHE Annual Meeting*, Miami Beach, FL. November 1995.

Jayawardena S.S. and McQuillen, J.B. "Microgravity two-phase flow at a pipe junction." paper 96-2070 presented at the 27th AIAA Fluid Dynamics Conference, New Orleans, LA., June, 1996.

Langbein, D. and Weislogel, M., "Dynamics of liquids in edges and corners (DYLCO)." *IML-2 Investigators Annual Meeting*, ESRIN, Frascati, Italy, Nov. 7-8, 1995.

Langbein, D. and Weislogel, M.M., "Dynamics of liquids in edges and corners." *2nd European Symposium Fluids in Space*, Naples, Italy, April, 1996.

Weislogel, M., "Isothermal capillary phenomena." *ZARM/Bremen University Colloquium Seminar Series*, Bremen, Germany, November 1995.

Weislogel, M., "Capillary flows: significance of the contact line boundary condition." *ZARM/Bremen University Open Forum Seminar*, Bremen, Germany, November 1995.

Zhang, N. and Chai, A.T., "Effects of evaporation on thermocapillary flows in liquid thin layer." *4th International Symposium on Heat Transfer*, Beijing, China, October 4 - 11, 1996.

Zhang, N. and Chai, A.T., "Marangoni-Benard convection in an evaporating liquid thin layer." *4th International Symposium on Heat Transfer*, October 4 - 11, 1996, Beijing, China.

Solute Nucleation and Growth in Supercritical Fluid Mixtures

PRINCIPAL INVESTIGATOR: Dr. Gregory T. Smedley

California Institute of Technology (Caltech)

CO-INVESTIGATORS:

Wilemski, G.

Lawrence Livermore National Laboratory

Task Objective:

We plan to study the nucleation and growth of naphthalene in supercritical carbon dioxide. This system is chosen due to the accessibility of relevant experimental conditions in the laboratory, and the importance of CO₂ in many technological applications. The strong dependence of solubility on pressure in supercritical fluids enables us to decouple the nucleation and growth processes so they may be studied independently.

Task Description:

1. Define experimental parameters for supercritical expansion processes. These include thermodynamic process paths, equilibrium solubilities, particle size and growth rate estimates.
2. Determine solid particle nucleation and growth rates from Mie scattering and extinction measurements.
3. Analyze experimental data, including phenomenological analytical modeling as necessary.
4. Develop and recommend a flight experiment design based on the results of the ground-based experiment.

Task Significance:

The experiments will employ rapid, but controlled, changes of the supercritical fluid pressure to vary the thermodynamic state of the fluid from a stable condition to one favoring solute nucleation and then to one fostering only solute particle growth. By using optical methods to measure the number of particles formed and their size, we can determine nucleation rates and growth rates at various thermodynamic conditions. Since the rates of nucleation of solid particles have never before been measured under these conditions, the data to be obtained will be invaluable for testing and improving nucleation theory as well as for guiding the design of a space-based experiment. One of the most important goals of the ground-based experiment will be to evaluate the effects of gravity on the measured nucleation rates. Because the density of near-supercritical and supercritical fluids varies rapidly with pressure, gravity may induce nonuniform conditions in the experimental fluid mixtures. This would make accurate ground-based measurements difficult if not impossible.

The results of this experimental/analytical work can be applied to the understanding of nucleation and growth problems found in many fields such as biotechnology (protein crystal growth), material science (sintered alloys), and analytical chemistry (supercritical fluid extraction and chromatography).

Progress During FY 1996:

The focus of the second year of this project has been to model the expected nucleation and growth rates along thermodynamic process paths to determine those that are likely to be of greatest interest to the scientific objectives, to determine the optimal configuration of the light scattering optics for the apparatus, and to design an apparatus and suitable instrumentation. Model calculations of nucleation rates along expected isentropic expansion paths has shown that paths can be selected with appropriate starting conditions that will yield nucleation and growth rates that are within the reach of the apparatus. The calculations also showed that it was possible to select paths that would lead to significant growth within the very short nucleation period that would prevent the possibility of determining the size and number density of the particles. The model calculations therefore act as a guide to the selection of thermodynamic paths that are likely to produce results within the measurement capability of the apparatus. The ultimate determination of nucleation and growth rates; however, lies in the results of the measurements. Optical light scattering (Mie scattering) calculations were utilized to determine the range of measurable particle sizes and number densities that could be achieved within the mechanical constraints of the apparatus.

The apparatus design task required consideration of instrumentation sensitivity, apparatus effectiveness, and process path optimization to arrive at an acceptable compromise. The apparatus was designed to operate over temperatures from ambient to 80 degrees Celsius and pressures from vacuum to 17MPa (2500psi). Thermodynamic calculations indicated that the size of the rapid volume expansions necessary to span the supercritical operating envelope (31 to 65 degrees Celsius, 7 to 17MPa) were about 30% of the initial volume. The determination of this small volume expansion requirement led to the consideration of an apparatus that employs a thin diaphragm, rather than the original moving piston, to create the desired expansions and recompressions. The supercritical mixture is contained on one side of the diaphragm and an expansion and recompression volume are connected to the opposite side through a pair of fast acting valves. Opening the valves in sequence produces first a rapid expansion and then a rapid recompression. Fiber optics with integral collimating lenses will be used for the light scattering and extinction measurements. All appropriate sensors and optics have been procured, the design is complete, and the apparatus is being machined. The operational success of the apparatus hinges on two critical technologies: (1) the fast acting valves must produce the required rapid opening times and (2) the flexible diaphragm must operate as expected without bursting. Fast acting valves that met the requirements of the apparatus were not commercially available and had to be designed to achieve less than 1msec opening times with a large orifice diameter (5mm) and zero leakage. The laboratory where the experiments will be conducted is being set up to operate and house the apparatus.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 8/94 EXPIRATION: 8/97

PROJECT IDENTIFICATION: 962-24-05-69

NASA CONTRACT NO.: NAS3-272

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Smedley, G.T., Wilemski, G., Rawlins, W.T., Oakes, D.B., Joshi, P., and Durgin, W.W., "Solute nucleation and growth in supercritical fluid mixtures." Third Microgravity Fluid Physics Conference, Cleveland, OH, June 13-15, 1996.

Behavior of Unsteady Thermocapillary Flows

PRINCIPAL INVESTIGATOR: Prof. Marc K. Smith

Georgia Institute of Technology

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective is to investigate thermocapillary instabilities to provide an understanding of the mechanisms of flow instabilities. The study will also indicate how well the stability theory results for simple geometries apply to the behavior of thermocapillary flows in more complex geometries.

Task Description:

The research approach consists of both a theoretical and an experimental effort. Two nonlinear analytical models for study of post-critical thermocapillary flows in a bounded domain will be constructed as part of the theoretical work. The models will be used to explore the effects of Pr , interfacial heat transfer, domain size, 3-D disturbances, and interfacial deformation on system flow stability. An experimental investigation of thermocapillary instabilities of opaque, low Pr and high Pr fluids will be also be performed.

Task Significance:

This understanding will assist fluid system designers optimize system designs in which thermocapillary flows are important.

Progress During FY 1996:

Steady, two-dimensional flow states in a thin liquid layer contained in a finite rectangular cavity have been found in terms of the free-surface deformation over a finite range of capillary numbers. This range is bounded from above by a limit point value of the capillary number. Below this value, two solution branches occur: a high-deformation branch; and a low-deformation branch. The high-deformation solution branch is unstable and the layer tends toward either the stable, lower-branch solution, or to film rupture. Above the limit-point value, no steady-state flows exist. The layer seems to progress towards a ruptured-film state at the hot end of the film.

The influence of inertia in the liquid layer was examine by allowing for a flow with a large Reynolds number. The resulting leading-order momentum equation was solved approximately using an integral technique. A parabolic longitudinal velocity was assumed, it was substituted into the momentum equation, and the result was averaged over the thickness of the layer. The resulting momentum equation, together with a mass conservation equation was solved using the same pseudo-spectral techniques used for the viscous-dominated case. The results show that the effect of inertia in the liquid is to reduce the free-surface deformation for a given capillary number and to increase the value of the limit point capillary number. The upper-branch solution is still unstable and the lower-branch solution is stable. However, at low capillary numbers, the preferred disturbance mode for the lower branch is oscillatory when inertia is included. We have shown that for small enough capillary numbers, the free surface behaves like a damped vibrating beam.

Steady, axisymmetric flow states have also been found in terms of free-surface deformation over a finite range of capillary numbers for flows occurring in two additional geometries: a wide, flat annular cavity with a flat free-surface; and a shallow cylindrical cavity with a cylindrical free-surface. The basic flow states in the annular cavity are similar to the rectangular cavity discussed earlier. The effect of azimuthal curvature is to destabilize the film when the inner radius of the film is large. This means that the limit-point capillary number is decreased. However, when the inner radius is small enough, the film is stabilized significantly. Near the point where the inner radius goes to zero, the film is completely stabilized. In this situation, a steady-state film profile is possible for all values of the capillary number. The limit-point capillary number goes off to infinity.

In a shallow cylindrical cavity, the inherent cylindrical curvature of the free surface always has a destabilizing effect on the film flow. The extra destabilization is due to a Rayleigh capillary instability associated with this geometry.

Our future work will be to include the effect of liquid inertia in the calculations for the cylindrical cavity. The stabilization effect of inertia may offset the destabilization effect inherent in the cylindrical geometry and result in a stable film flow on the cylinder. This type of behavior could be very significant in terms of understanding the stability of thermocapillary flow in liquid bridges and in the float-zone crystal growth process.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 1/93 **EXPIRATION:** 5/96**PROJECT IDENTIFICATION:** 962-24-05-62**NASA CONTRACT NO.:** NAG3-145**RESPONSIBLE CENTER:** LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Vrane, D.R. and Smith, M.K. "The influence of domain curvature on the stability of viscously-dominated thermocapillary flows." Advances in Multi-Fluid Flows, Proceedings of the AMS-IMS-SIAM Joint Summer Research Conference on Multi-Fluid Flows and Interfacial Instabilities, 1996.

Vrane, D.R. and Smith, M.K., "The influence of domain curvature on the stability of viscously-dominated thermocapillary flows." Forth-Eighth Meeting of the American Physical Society - Division of Fluid Dynamics, Irvine, CA, November 19-21, 1995.

The Development of Novel, High-Flux, Heat Transfer Cells for Thermal Control in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Marc K. Smith

Georgia Institute of Technology

CO-INVESTIGATORS:

Glezer, A.

Georgia Institute of Technology

Task Objective:

The objective is to investigate the fundamental fluid mechanics and heat transfer processes involved in "Heat Transfer Cells" (HTC's) for microgravity applications. An operational prototype of a HTC that uses droplet evaporation for cooling will be developed.

Task Description:

Experimental and numerical work will be carried out to investigate the fluid flow and heat transfer processes and to develop the HTC. Vibration induced droplet atomization (VIDA) technology will be developed to use in the HTC to burst fluid drops into a shower of smaller ones.

Task Significance:

Devices such as HTC's are important to meet the future needs of thermal management and control in space applications. These self-contained HTC's are capable of transferring much larger heat fluxes than a conventional heat pipe. These units could be operated in parallel or in series, to achieve high heat-flux capacities or efficient heat transfer over long distances.

Progress During FY 1996:

This is a new grant starting in FY96. Data from the preliminary experiments that have been done over the past year in anticipation of this award are being analyzed. This work was presented at the American Physical Society meeting this year.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 9/96 EXPIRATION: 9/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-194

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Smith, M. and Glezer, A., "The development of novel, high-flux, heat transfer cells for thermal control in microgravity." Proceedings of Third Microgravity Fluid Physics Conference, Cleveland OH, June 13-15, 1996.

Presentations

James, A., Smith, M.K., and Glezer, A. "The explosive ejection of small droplets from a liquid-gas interface." American Physical Society, Division of Fluid Dynamics, November 24-26, 1996.

Dynamics of the Molten Contact Line

PRINCIPAL INVESTIGATOR: Dr. Ain A. Sonin

Massachusetts Institute of Technology (MIT)

CO-INVESTIGATORS:

Patera, A.T.

Massachusetts Institute of Technology

Qiu, T.

Massachusetts Institute of Technology

Task Objective:

The purpose of the proposed work is to develop, based on both experiments and theory, a fundamental understanding of the dynamic processes that occur when a hot, molten droplet impact on a cold solid, spreads partly over it by capillary action, and freezes. These processes are of particular importance in evolving methods of materials processing, where interest centers on microscale droplets which are so small that gravitational effects are negligible and capillary forces dominate. Microgravity offers ideal conditions for studying these phenomena because it allows experimental simulation of microscale conditions at scales large enough for proper instrumentation.

While a great deal of research has been published during the last two decades on the capillarity controlled deposition and spreading of an ordinary liquid on a solid surface, the spreading of molten materials remains unexplored. The key phenomena that are not understood are (a) the dynamics of a molten liquid front's advance over a cold surface under capillarity-driven conditions, and (b) the mechanism of the molten contact line's arrest by freezing. These phenomena turn out to be surprisingly complex, and a fundamental understanding is lacking. The proposed work will result in generic methods for predicting the deposition, spreading, arrest and solidification, and thus the final shapes of molten microscale droplets deposited on cold substrates.

Task Description:

The work has five proposed parts:

- (1) basic laboratory studies using deposition experiments with small molten droplets,
- (2) experimental investigation of the dynamics of the molten contact line on a laboratory system with controlled forced spreading,
- (3) development and testing of a new temperature measurement technique with microscale resolution and microsecond time response,
- (4) tests under microgravity conditions, where simulation of microscale drops can be done at a scale large enough for detailed measurements using the techniques of (3), and
- (5) theoretical work to develop a realistic model for contact line arrest and solidification.

The key theoretical problem is the resolution of a mathematical singularity which occurs in the thermal contact line problem.

Task Significance:

The deposition and solidification of molten microdrops is increasingly important in new methods of materials processing. One application which will require the results of this research in order to be commercially developed is 'digital microfabrication', or fabrication of three-dimensional objects microdrop under complete computer control much in the same way as two-dimensional hard copy is obtained in ink-jet printing. Molten microdrops 50 μ m in diameter can be deposited accurately at high rates, each droplet solidifying by heat loss after it lands, and very finely featured objects of quite arbitrary three-dimensional shape can be produced.

To be able to program a fabrication process on a computer, however, it is necessary first of all to know how to control the shape of the basic "building block" in the process, that is, the shape that a molten microdrops take after it lands on a cooled surface, spreads partly over it, and solidifies. This shape is determined by the impact velocity, material properties, the local temperature of the material on which the droplet lands (which in turn affected by deposition rate), etcetera. Virtually no information is available on molten droplet deposition under conditions suitable for precise microfabrication of objects. This research work will provide a fundamental knowledge base for

this technology, and show what operating conditions will be needed and how they depend on materials properties. This information is required not only for process control, but also for industry to assess potential new applications and decide whether to invest in developing the required new technology.

The unsolved fundamental problems which this work also addresses play key roles in other current applications, including materials processing by rapid solidification, near-net-shape fabrication of parts, and crystal growth.

Progress During FY 1996:

This program began near the end of FY 1996. Experiments are in progress on the molten droplet deposition dynamics and contact line arrest, and work has begun on developing instrumentation for the local temperature measurements in the region near the moving contact line.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/96 EXPIRATION: 5/97

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-184

RESPONSIBLE CENTER: LeRC

Marangoni Effects on Drop Deformation and Break-Up in an Extensional Flow: The Role of Surfactant Physical Chemistry

PRINCIPAL INVESTIGATOR: Dr. Kathleen J. Stebe

Johns Hopkins University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to study the role of the physical chemistry of surfactants in determining the stress conditions at the interface of a droplet deforming in an extensional flow. Both theoretical modeling and experiments will be performed to establish a framework for the prediction and control of the droplet dynamics.

Task Description:

The proper modeling of the effects of surfactants requires an understanding of the surfactant thermodynamics and kinetics. The equilibrium and dynamic behavior of well characterized surfactants and their equations of state will be used in determining the dynamics of drops in an extensional flow. Numerical simulations using the boundary element method will be performed to predict the shape and flow fields in the drop, starting from an initially spherical shape. The calculations will be performed until a steady shape is attained or the drop fragments.

Experiments in a four roll mill will be performed in the presence of surfactants. The accuracy of the theoretical model in predicting the evolution of the shape of the drop and its break-up will be tested.

Task Significance:

Surfactants are present as contaminants, components or additives in nearly all fluids. This research effort emphasizes the effects of their physical chemistry (size, orientation and affinity) on how they affect the transfer of momentum at fluid interfaces. This will lead to improved prediction and control of the dynamics of fluid interfaces. Surfactants are extensively used in industrial applications such as enhanced oil recovery, food and beverage processing, emulsions, pharmaceuticals and cosmetics and many chemical processes.

Progress During FY 1996:

This research program has been initiated in July 1996. The tasks that are planned to be performed in the first year are (i) Construction of the four-roller mill and experimental characterization of the surfactants that will be studied (ii) Complete the theoretical study of two types of surfactant transport, viz., insoluble surfactants and adsorption-desorption controlled regimes.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/96 EXPIRATION: 7/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-192

RESPONSIBLE CENTER: LeRC

Flow-Influenced Shape Stability: Breakup in Low Gravity

PRINCIPAL INVESTIGATOR: Prof. Paul H. Steen

Cornell University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

1. Understand the influence in low gravity of flow on interface shape. For example, document and control the influence of axial flow on the Plateau-Rayleigh instability of a liquid bridge.
2. Extend the ground-based density-matching technique of low gravity simulation to situations with flow; i.e., develop Plateau chamber experiments for which flow can be controlled.

Task Description:

The configuration of a liquid held by surface tension under low gravity is susceptible to significant modification by liquid motion. Motion destabilizes in general but there are narrow circumstances where motion can stabilize. We identify these circumstances theoretically, by solving linear and nonlinear stability problems, and try to locate them in experiments conducted with a dynamic Plateau apparatus. Overall, the goal is an understanding of the influence of flow on shape.

Task Significance:

Containerless containment of liquids by surface tension has broad importance in low gravity. For space vehicles, the behavior of liquid/gas interfaces is crucial to successful liquid management systems. In microgravity science, free interfaces are exploited in various applications. Examples include float-zone crystal growth, phase separation near the critical point of liquid mixtures (spinodal decomposition) and quenching of miscibility gap molten metal alloys. In some cases, it is desired to stabilize the capillary instability while in others it is desired to induce capillary breakup. In all cases, understanding the stability of interface shape in the presence of liquid motion is central.

Predicting the way an object breaks from one piece into two or more pieces is arguably the oldest unsolved problem in engineering. We study this question in the simple context of the pinchoff of a film bridge. Our work has practical implications for many industrial and natural phenomena.

Progress During FY 1996:

Both analytical/numerical and experimental approaches are employed.

Stability analyses include linear and nonlinear techniques. The linear stability approach has been used to analyze the shape stability of a cylindrical interface containing axial shear flows, both isothermally- and thermocapillary-driven. Computational feasibility currently limits this approach to base states that are separable flows, effectively, the axial-infinite interfaces. It is now well known that infinite cylindrical interfaces can be stabilized. For finite interfaces an alternate approach is needed. In the limit of no motion, minima of the free energy functional are obtained using the calculus of variations supplemented by numerical branch-tracing. For weak motion (creeping flow), we extend this approach using a modified functional. Near the singularity represented by the Plateau-Rayleigh limit, bifurcation theory using Liapunov-Schmidt reduction is a natural tool for the solution of the appropriate nonlinear Euler-Lagrange equation. All these analytical/numerical tools lend themselves to understanding the physics of stability in terms of simple competition mechanisms.

As for the experimental approach, a dynamic Plateau chamber has been built and is used to study liquid bridges held captive by rod-ends and embedded in an axial surrounding flow. Theory has guided the experiments to a particular window in parameter space. Such guidance is crucial since interesting stabilization effects occur over narrow parameter ranges for this problem.

Progress on theory

We have found a self-similar solution for the inviscid pinchoff of a film bridge. A combination of computational and analytical attack has been successful.

Progress on experiment

The experimental apparatus is being overhauled to improve measurement and control of temperatures, flow rates and digital imaging.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 1/93 EXPIRATION: 1/96

PROJECT IDENTIFICATION: 962-24-05-57

NASA CONTRACT No.: NAG3-801

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Chen, Y.-J. and Steen, P.H., Suppression of the capillary instability in the Rayleigh-Taylor slot problem. Phys. Fluids 8, 1, 97-102 (1996).

Lowry, B.J., and Steen, P.H., Shape stability of slender liquid bridges in axial flows. J. Fluid Mech. , (accepted 1996).

Proceedings

Chen, Y.-J. and Steen, P. H., "Stabilizing interfaces of finite extent with flow induced by thermal convection, in advances in multi-fluid flows." SIAM publishers, 211-18,1996.

Chen, Y.-J. and Steen, P. H., "Influence of thermocapillary flow on capillary stability: long float-zones in low gravity." Proceedings of Third Microgravity Fluid Physics Conference, Cleveland OH, June 13-15, 1996.

Presentations

Steen, Paul H., "Inviscid capillary breakup: collapse of the soap-film bridge." University of Dresden, Dresden, GERMANY, 3 May 1996.

Steen, Paul H., "Inviscid capillary breakup: collapse of the soap-film bridge." ESPCI Paris, Paris, FRANCE, May 24, 1996.

Stability of Shapes Held by Surface Tension and Subjected to Flow

PRINCIPAL INVESTIGATOR: Prof. Paul H. Steen

Cornell University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this study is to predict, measure, and control instabilities that occur in liquid bridges and during the formation of bubbles and droplets at a nozzle.

Task Description:

For the liquid bridge, use 'dynamic balancing' (Plateau tank with fluid flow to cancel density imbalances and thereby simulate zero gravity) to characterize Bond number drifts with temperature in the Plateau apparatus.

For the liquid bridge, in the light of the theoretical results (non-linear region, steady flow), carry out experiments in the range of stabilization that is 5-10% beyond the Plateau-Rayleigh limit.

Design and construct a prototype glove box experiment, based on the 'dynamic balancing' principle, to use the liquid bridge shape as a g-level meter.

Carry out experiments subjecting liquid bridges to oscillating flows to achieve fluid bridges 50-100% longer than the Plateau-Rayleigh limit, using real-time image processing and feed-back control.

Carry out experiments of bubbling argon into molten aluminum through different nozzle materials and designs, and thus study the effects of wetting characteristics, and contact-line motion.

In the dynamic Plateau chamber, carry out 1) experiments to test the theory for bubbles and fixed-contact line, and 2) experiments to compare with the Argon - molten Aluminum experiments.

Carry out complementary theoretical studies on the various stability experiments described above.

Task Significance:

This experimental and theoretical program, (like those studies on the effect of acoustic, magnetic, and electrical fields), aims to understand the effect of flow on liquid/gas interfaces, fundamental to many issues in materials processing and liquid management in low gravity.

These studies on fluid bridges and bubbles/drops are likely to shed light on many fundamental questions of interface stability, the role of wetting and contact line motion in the 3-phase region (solid nozzle, liquid metal, and the gas), and surface tension measurements of molten metals.

Progress During FY 1996:

This is a new grant starting in FY96. The first task has been to upgrade the tolerances to which the observables in the dynamic plateau apparatus have been monitored and controlled. For example, the goal is to control temperature to a fraction of a degree Kelvin across the apparatus and in time over a 12 hour interval. This has involved redesign of parts of the apparatus to incorporate temperature probes, enhanced data logging, and automation of the digital image processing technique. Benchmarking the improvements using theory has been a crucial metric.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 2

TASK INITIATION: 5/96 EXPIRATION: 4/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-185

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Chen, Y.-J. and Steen, P. H., "Influence of thermocapillary flow on capillary stability: long float-zones in low gravity." Proceedings of the Third Microgravity Fluid Physics Conference, Cleveland OH, June 13-15, 1996.

Presentations

Steen, Paul H., "Inviscid capillary breakup: collapse of the soap-film bridges." University of Dresden, Dresden, Germany, May 3, 1996.

Steen, Paul H., "Inviscid capillary breakup: collapse of the soap-film bridges." ESPCI Paris, Paris, France, May 24, 1996.

Interactions of Bubbles and Drops in a Temperature Gradient

PRINCIPAL INVESTIGATOR: Prof. R. S. Subramanian

Clarkson University

CO-INVESTIGATORS:

Balasubramaniam, R.

NASA Lewis Research Center (LeRC)

Task Objective:

The objective of this research is to study the interactions of bubbles and drops in the presence of a temperature gradient in the continuous phase. The goal is to understand how the presence of a neighboring drop alters the motion of a test drop and whether the two drops coalesce. Both theoretical and experimental research is planned on the interactions of drops with each other or with a neighboring boundary.

Task Description:

The emphasis of the initial effort is on the design, fabrication and set up of the experimental hardware, and to check its performance. Experiments will then be performed using a suitably chosen liquid-liquid system such that the drops sink due to buoyancy. The drops will be subjected to a vertical temperature gradient; thermocapillary forces will then cause the drops to move upwards. Initially experiments will be performed with single drops and the results will be compared with existing theory. Subsequent experiments will focus on drop interactions.

Task Significance:

This research attempts to provide important information on interactions of drops, i.e., how the presence of a drop affects the motion of another, in a medium where the temperature is non-uniform. Primary emphasis is on thermocapillary flow, thereby the research is more applicable to drop interactions under reduced gravity. The nature of these pairwise interactions determines whether the drops speed up or slow down as they approach each other and whether they collide or glide past each other. Pairwise interaction data are very useful in models that track coalescence in a many drop dispersion.

Progress During FY 1996:

Data were gathered on several pairs of drops moving in a temperature gradient of approximate value 1.25 K/mm. The drops are of diethyl maleate and the continuous phase is propanediol. Two orthogonal views of the motion were obtained since the actual trajectories are three dimensional. After considerable effort all of the data from the two views were analyzed to obtain information on position versus time for both of the drops. A task that still remains is to compare the data on pair interactions with predictions from linear theoretical models and the results obtained for isolated drops at non-negligible values of the Marangoni number. The latter comparison will gauge the extent of the interaction between members of the pair.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 3/93 EXPIRATION: 2/96

PROJECT IDENTIFICATION: 962-24-05-58

NASA CONTRACT NO.: NAG3-147

RESPONSIBLE CENTER: LeRC

Instability in Surface-Tension-Driven Benard Convection

PRINCIPAL INVESTIGATOR: Prof. Harry L. Swinney

University of Texas, Austin

CO-INVESTIGATORS:

McCormick, W.D.

University of Texas, Austin

Swift, J.B.

University of Texas, Austin

Task Objective:

The objectives of this work are to investigate and characterize the primary and secondary instabilities in surface-tension-driven (Benard-Marangoni) convection in laboratory experiments and simulations.

Task Description:

Noninvasive optical techniques (including shadowgraph and infrared imaging) were used to study patterns formed in surface-tension-driven convection for a wide range of vertical temperature gradients imposed on the liquid layers. The long wavelength ($k = 0$) instability was examined in linear and nonlinear stability analyses and numerical simulations, and the results of the calculations were compared quantitatively with laboratory experiments.

Task Significance:

Surface tension force dominates many physical processes in space and strongly influences many important problems on Earth, such as manufacturing (e.g., welding, coatings); industrial heating, cooling, and mixing (e.g., thin film heat exchangers); and the processing of commercially important materials (e.g., electronic or biological crystal growth). The present work seeks to elucidate the basic mechanisms of instability and to determine and characterize the different types of instabilities that occur in surface-tension driven systems, and to refine and develop laboratory techniques that can be used for studying surface tension driven phenomena in space and terrestrial applications.

Progress During FY 1996:

• High Marangoni number studies:

We have studied Marangoni convection for very large Marangoni number (very large vertical temperature gradients). The squares we reported in FY 1996 are found to lose stability to a disordered state, whose cells continue to grow in size with increased Marangoni number. We are investigating an analogy between this disordered state and work on soap bubbles and magnetic bubbles.

• Long-wavelength two-layer model: development and comparison with experiment:

We have developed a two-layer model for instability at long wavelength ($k \rightarrow 0$) that provides better agreement with our experimental observations than the previously developed single layer model. We are currently testing a prediction by this two-layer model of a new type of long-wavelength primary instability.

• Investigation of role of spatial nonuniformity:

We have studied theoretically and numerically the effect of small nonuniformities upon the onset of the long-wavelength instability. We have found that even a 1% nonuniformity can cause significant (40%) deformation of the liquid-air interface before onset of the instability. In addition, the nonuniformity causes onset earlier than predicted by linear stability theory.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 1

TASK INITIATION: 12/92 EXPIRATION: 11/95

PROJECT IDENTIFICATION: 962-24-05-41

NASA CONTRACT NO.: NAG3-138

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Schatz, M.F., VanHook, S.J., McCormick, W.D., Swift, J.B., and Swinney, H.L., Onset of surface-tension-driven Benard convection. Phys. Rev. Lett., 75, 1938-1941 (October 1995).

VanHook, S.J., Schatz, M.F., McCormick, W.D., Swift, J.B., and Swinney, H.L., Long-wavelength instability in surface-tension-driven Benard convection. Phys. Rev. Lett., 75. 4397-4400 (October 1995).

Proceedings

Schatz, M.F., VanHook, S.J., McCormick, W.D., Swift, J.B., and Swinney, H.L., "Experimental control of thermocapillary convection in a liquid bridge." Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, 1996.

VanHook, S.J., Schatz, M.F., McCormick, W.D., Swift, J.B. and Swinney, H.L., "Long-wavelength instability in Marangoni convection." Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, 1996.

Instabilities in Surface-Tension-Driven Convection

PRINCIPAL INVESTIGATOR: Prof. Harry L. Swinney

University of Texas at Austin

CO-INVESTIGATORS:

Schatz, M.

University of Texas at Austin

McCormick, W.D.

University of Texas at Austin

Swift, J.B.

University of Texas at Austin

Task Objective:

The objectives of this work are to investigate the primary and secondary instabilities in surface-tension-driven convection in terrestrial experiments on thin fluid layers heated from below. The conditions are chosen to yield insight on surface-tension-driven convection in microgravity, where buoyancy plays a negligible role.

Task Description:

Laboratory experiments, numerical simulations, and theoretical analyses will be conducted to elucidate instabilities in liquids with an imposed temperature gradient. Different geometries to be investigated include the classical Benard system, a container of liquid heated from below. A second geometry will be a liquid bridge between an hot upper cylinder and a cool lower cylinder. Measurements of the entire temperature field of the liquid surface will be compared with analyses and numerical simulations.

Task Significance:

Surface tension force dominates many physical processes in space and strongly influences many important problems on Earth, such as manufacturing (e.g., welding, coatings); industrial heating, cooling, and mixing (e.g., thin film heat exchangers); and the processing of commercially important materials (e.g., electronic or biological crystal growth). The present work seeks to elucidate the basic mechanisms of instability and to determine and characterize the different types of instabilities that occur in surface-tension-driven systems, and to refine and develop laboratory techniques that can be used for studying surface tension driven phenomena in space and terrestrial applications.

Progress During FY 1996:

- Secondary and higher instabilities in surface-tension-driven convection:

Our laboratory studies of convection in a fluid layer heated from below reveal a secondary transition in the convection pattern, from the hexagonal pattern formed at the initial instability to a state with an array of square convection cells. With yet higher Marangoni number (i.e., with a larger vertical temperature difference across the liquid layer), the squares lose stability to a disordered state whose cells continue to grow in size as the Marangoni number is increased further. We are investigating an analogy between this disordered state and work on soap bubbles and magnetic bubbles.

- Long-wavelength instability: comparison with experiment and a model:

We have developed a two-layer model for instability in surface-tension-driven convection at long wavelength ($k \rightarrow 0$). This instability occurs in liquid layers that are sufficiently thin and viscous. A comparison of our detailed laboratory studies of this instability shows that our two-layer model provides better description of the instability phenomenon than the previously developed single layer model. In addition, the two layer model predicts a new type of long-wavelength primary instability; we will now search for this instability.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT No.: NAG3-183

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Schatz, M.F., VanHook, S.J., McCormick, W.D. Swift, J.B., and Swinney, H.L., "Experimental control of thermocapillary convection in a liquid bridge." Proceedings of the Third Microgravity Fluid Physics Conference 1996.

VanHook, S.J., Schatz, M.F., McCormick, W.D., Swift, J.B., and Swinney, H.L. "Long-wavelength instability in Marangoni convection." Proceedings of the Proceedings of the Third Microgravity Fluid Physics Conference 1996.

Presentations

Swinney, H.L., "Nonlinear dynamics seminar and physics department colloquium." Universidad Nacional Autonoma Mexico, Mexico City, August 13-14, 1996.

Crystal Growth and Fluid Mechanics Problems in Directional Solidification

PRINCIPAL INVESTIGATOR: Prof. Saleh Tanveer

Ohio State University

CO-INVESTIGATORS:

Baker, G. R.

Ohio State University

Foster, M. R.

Ohio State University

Task Objective:

The objective of this program is the exploration of phenomena in directional solidification using mathematical modeling and computing to increase our understanding in two principal areas: 1) Evolution of dendritic fingers, which arise in a wide variety of problems involving solidification out of an undercooled melt. 2) Analysis and optimization of the performance of a vertical Bridgman furnace used to process dilute binary alloys.

Task Description:

Our basic approach to these problems is their careful mathematical formulation followed by use of a variety of mathematical and numerical techniques that allow solution of the complex problems. In the case of item (1) of the objectives indicated above, dendrites often grow in settings in which the proper measure of the surface energy is very small, and that leads to a mathematical problem for the dendrite's evolution that is not well posed. We utilize a technique used previously by Tanveer (Phil. Trans. Roy. Soc. Lond A 343, 1993) in Hele-Shaw problems to describe the interfacial evolution. For item (2), we use two approaches--one involving the use of asymptotic methods at large Rayleigh numbers, and the second utilizing a fully numerical approach to solve the problem computationally.

Task Significance:

The production of a number of binary alloys that are used in a variety of applications in the electronics industry involves solidification processes of one form or another. Clearly in such production, economic viability requires production rates to be as high as possible. Unfortunately, rapid solidification often leads to cellular structures at the melt-crystalline interface and ultimately to dendritic structures. Better fundamental understanding of dendritic growth processes is a necessary first step in their control and/or suppression. Even at lower solidification rates, non-uniformity in the crystalline product can lead to large portions of the crystal being discarded. The detailed mathematical analysis of the Bridgman furnace, used for the formation of many such alloys, and in particular the determination of optimized performance parameters, can lead to much higher efficiency of the process, in the sense that there would be less waste.

Progress During FY 1996:

This project has been completed as of June 1996 and will continue under Task ID Number 962-24-00, beginning June, 1996. A complete progress is in that report.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 1/93 EXPIRATION: 12/96

PROJECT IDENTIFICATION: 962-24-05-53

NASA CONTRACT No.: NAS1-186

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Siegel, M. and Tanveer, S., Singular perturbation of smoothly evolving Hele-Shaw solutions. Physical Review Letters, (October 1996).

Presentations

Baker, G. and Koester, G., "Steady-state computations in a vertical Bridgman Furnace." American Physical Society Division of Fluid Dynamics Meeting, Irvine, CA, November 1995.

Foster, M.R., "Boundary-layer theory for a vertical Bridgman device." American Physical Society Division of Fluid Dynamics Meeting, Irvine, CA, November 1995.

Kunka, M.D., Tanveer, S., and Foster, M.R., "Nonlinear evolution of the zero surface tension, small peclet number dendrites." American Physical Society Division of Fluid Dynamics Meeting, Irvine, CA, November, 1995.

Crystal Growth and Fluid Mechanics Problems in Directional Solidification

PRINCIPAL INVESTIGATOR: Prof. Saleh Tanveer

Ohio State University

CO-INVESTIGATORS:

Baker, G.R.

Ohio State University

Foster, M.R.

Ohio State University

Task Objective:

The objective of this program is the exploration of phenomena in directional solidification using mathematical modeling and computing to increase our understanding in two principal areas: (1) Evolution of dendritic fingers, which arise in a wide variety of problems involving solidification out of an undercooled melt. (2) Analysis and optimization of the performance of a vertical Bridgman furnace used to process dilute binary alloys.

Task Description:

Our basic approach to these problems is their careful mathematical formulation followed by use of a variety of mathematical and numerical techniques that allow solution of the complex problems. In the case of item (1) of the objectives indicated above, dendrites often grow in settings in which the proper measure of the surface energy is very small, and that leads to a mathematical problem for the dendrite's evolution that is not well posed. We utilize a technique used previously by Tanveer (*Phil. Trans. Roy. Soc. Lond A* **343**, 1993) in Hele-Shaw problems to describe the interfacial evolution. For item (2), we use two approaches—one involving the use of asymptotic methods at large Rayleigh numbers, and the second utilizing a fully numerical approach to solve the problem computationally.

Task Significance:

The production of a number of binary alloys that are used in a variety of applications in the electronics industry involves solidification processes of one form or another. Clearly in such production, economic viability requires production rates to be as high as possible. Unfortunately, rapid solidification often leads to cellular structures at the melt-crystalline interface and ultimately to dendritic structures. Better fundamental understanding of dendritic growth processes is a necessary first step in their control and/or suppression. Even at lower solidification rates, non-uniformity in the crystalline product can lead to large portions of the crystal being discarded. The detailed mathematical analysis of the Bridgman furnace, used for the formation of many such alloys, and in particular the determination of optimized performance parameters, can lead to much higher efficiency of the process, in the sense that there would be less waste.

Progress During FY 1996:

The tasks completed in FY 1996 are as follows:

1. Dendritic Crystal Growth. We have considered the time-evolving aspects of a 'one-sided' model for growth of dendritic finger in two dimensions. Our focus is almost exclusively restricted to small surface energy effects. It is to be noted that for a dendrite that has a nearly parabolic shape, surface energy effects are reduced further away from the tip due to decreasing curvature and this makes the small surface energy limit of obvious relevance. If the rate of growth is sufficiently slow (corresponding to small 'Peclet number', P), the smallness of P can be utilized to construct perturbation-style solutions. We utilize both analytical and numerical methods to shed light on this limiting dynamics. A sequence of three papers will ultimately report our findings.

In Part I [Item 5], we carry out a formal asymptotic expansion for small Peclet number, P , and determine where such an assumed expansion ceases to be consistent. For a dendrite that is initially parabolic far from the tip, there is a small zone near that tip in which the temperature obeys a Laplace equation, very much like a Hele-Shaw problem, but with different far-field conditions (Tanveer, *Phil. Trans. Roy. Soc. Lond A* **343**, 1993). When initial shape deviation is confined to the tip region, we find that so long as the elapsed time is not too long, the other portions of the dendrite remain nearly parabolic, and all of the evolution is confined to the tip region. We examine growth of initially localized disturbances, and for the linearized case, our results are in conformity with those of Barber,

Barbeiri & Langer (*Phys. Rev. A* 36, 1987), though we find that the disturbances do not remain localized later in time. We also formulate a corresponding nonlinear problem, involving now an integro-differential equation, whose solution is dramatically different from what turns out to be a misleading linearized result--which, among other things, gives an incorrect result for rate of growth of the disturbances. Our insight into this difficulty with the former results rests on the use of a complex, rather than real, mathematical domain. For small surface energy, this seems the only way of coming to grips with the reality of the dendritic growth in a mathematically rigorous setting.

In Part II, presently in preparation [Item 10], the Part-I restrictions to dynamical features for zero surface energy are relaxed, and we explore how the presence of small surface energy affects the dendritic growth. Again, only in the context of a complex-plane analysis can this analysis be properly done.

In Part III [Item 11], we identify and amplify a specific mechanism on how the limiting dynamics for small surface energy differs from the zero-surface-energy dynamics itself. We also consider effects of anisotropy on 'daughter singularities' in the complex plane. We find that, unlike the case of isotropic surface energy, for which the tip region never becomes steady in time, the 'daughter-singularity' impact time can theoretically predict the formation of a locally steady tip region. A scale analysis in conjunction with highly accurate computations supports the scalings in the context of a dendrite as well as the mathematically analogous Hele-Shaw flow with anisotropic surface tension. [See also Item 2]

2. Bridgman crystal growth. In addition to the results by the P.I on flow in a Bridgman furnace (Tanveer, *Phys Fluids* 6, 1994) we have considered the analytical limit of large but negative solutal Rayleigh number and have determined conditions for optimal heat transfer across the edges of the insulation zone in order to minimize material nonuniformity [Item 3]. We find through boundary-layer methods that relaxing the unrealistic no-stress conditions at the side wall imposed previously gives results for both large thermal and solutal Rayleigh number that agree with Tanveer's former results, even with the changed fluid boundary conditions. In addition, optimization is also found to be possible if the Rayleigh numbers are of comparable order [Item 4].

We now have a number of computational results as well. Our approach to the study of optimal operating conditions for a Bridgman device is divided into two parts. First, we seek steady-states in which the crystal grows steadily inside the insulation zone. We use Newton's method to solve the discrete system, and also suppose that the solution is a quasi-stationary state in that the top and bottom of the ampoule are assumed to be sufficiently far away as to have no effect on the local behavior near the interface and insulation zone. By computing solution branches as various physical parameters are varied, we have been able to identify optimal operating conditions which minimize the radial material segregation [Item 9]. Second, we use a transient study to verify that a steady state can actually be achieved in a reasonable amount of time, and that the steady state will persist long enough to grow a crystal with desirable qualities over a sufficient length. We have found a special boundary condition for the top and bottom of the computational grid that simulates accurately the desired far-field behavior for an infinitely long ampoule. Thus we are able to compare the transient motion of the interface when the ampoule is infinitely long with an ampoule of finite length. We have confirmed the expectation that the side-wall Biot numbers play a crucial role in determining when an ampoule is long enough so that the interface will grow steadily without feeling the influence of the conditions at the top and bottom of the ampoule.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-194

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Siegel, M. and Tanveer, S., Singular perturbation of smoothly evolving Hele-Shaw solutions. *Physical Review Letters*, (1996).

Presentations

Baker, G.R. and Koester, G., "Steady-state computations in a vertical Bridgman furnace." American Physical Society Division of Fluid Dynamics Meeting, Irvine, CA, November 1995.

Foster, M.R., "Boundary-layer theory for a vertical Bridgman device." American Physical Society Division of Fluid Dynamics Meeting, Irvine. CA, November 1995.

Kunka., M.D., Tanveer, S., and Foster, M.R., "Nonlinear evolution of the zero surface tension, small Peclet number dendrites." American Physical Society Division of Fluid Dynamics Meeting, Irvine. CA., November 1995.

Microgravity Effects on Transendothelial Transport

PRINCIPAL INVESTIGATOR: Dr. John M. Tarbell

Pennsylvania State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The endothelial cell (EC) layer which lines blood vessels from the aorta to the capillaries provides the principal barrier to transport of water and solutes between blood and underlying tissue. Endothelial cells are continuously exposed to mechanical shearing force (shear stress) and normal force (pressure) imposed by flowing blood on their surfaces, and they are adapted to this mechanical environment. When the cardiovascular system is exposed to microgravity, the mechanical environment of endothelial cells is perturbed drastically and the transport properties of EC layers are altered in response. We have shown recently that step changes in shear stress have an acute effect on transport properties of EC layers in a cell culture model, and several recent studies in different vessels of live animals have confirmed the shear-dependent transport properties of the endothelium.

The hypothesis is that alterations in mechanical forces induced by microgravity and their resultant influence on transendothelial transport of water and solutes are, in large measure, responsible for the characteristic cephalad fluid shift observed in humans experiencing microgravity. To study the effects of altered mechanical forces on transendothelial transport and to test pharmacologic agents as counter measures to microgravity induced fluid shifts we propose ground-based studies using well defined cell culture models.

Task Description:

The specific questions to be addressed in this research are:

1. How do alterations in hemodynamic forces (pressure and wall shear stress) affect transendothelial water and protein fluxes?
2. What biochemical pathways mediate the influence of pressure and shear stress on endothelial transport properties?
3. Can the transport properties of endothelial monolayers be manipulated by pharmacologic agents in the hemodynamic environment of microgravity?

The proposed studies will provide the first direct understanding of the effects of mechanical perturbations induced by microgravity on the transport properties of the vascular system. The studies can be extended to animals and humans on the ground or in space and could ultimately lead to effective countermeasures to fluid shifts.

Task Significance:

Representative arterial endothelial cells and microvascular endothelial cells will be cultured on polycarbonate filters and exposed to controlled pressure and shear forces in a unique rotating disk device which was designed and built at Penn State University. Changes in mechanical forces induced by microgravity will be simulated and measured using this system. In addition, acute changes in endothelial transport properties (albumin permeability and hydraulic conductivity) will be measured.

The role of important second messenger systems known to be activated by changes in shear stress (cAMP, cGMP, Ca²⁺) which are coupled to the EC plasma membrane through G-protein-dependent receptors will be probed with various inhibitors to manipulate the mechanical force-dependent responses of EC transport properties. The role of the cytoskeleton, which distributes mechanical forces throughout the cell, will also be assessed with specific agents known to disrupt the major components of the cytoskeleton.

EC Monolayers will be exposed to microgravity hemodynamics using the rotating disk apparatus, while measuring the response of transport properties in the presence of the proper doses of pharmacological agents. Drugs which

affect the second messenger systems described under question 2 will be considered. Drugs which can counteract the affects of microgravity on EC transport may be useful as countermeasures to cephalad fluid shift when applied regionally using modern drug delivery technologies.

Progress During FY 1996:

This grant was newly awarded in May 1996. The process of hiring graduate students and ordering equipment has been completed. Experiment hardware is now in the initial assembly phase.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 2
PhD Students: 0

TASK INITIATION: 5/96 **EXPIRATION:** 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-187

RESPONSIBLE CENTER: LeRC

Oscillatory/Chaotic Thermocapillary Flow Induced by Radiant Heating

PRINCIPAL INVESTIGATOR: Dr. Robert L. Thompson

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

DeWitt, K.
Hsieh, K.
Van Zandt, D.University of Toledo
NYMA, Inc.
ADF

Task Objective:

The main objective of the research is to study the oscillatory and chaotic thermocapillary flows induced by radiant heating of the free surface of a high Prandtl number fluid. Both ground-based experiments and numerical analysis will be conducted to study effect of heating level (supplied by CO₂ laser), surface shape, aspect ratio, and Prandtl number on the conditions for transition from steady to oscillatory flows and then to chaotic flows. In the experiments, flow structures will be observed using a flow visualization technique and temperature distribution on the free surface will be measured using an infrared (IR) imager. Numerical results will be compared with experimental data.

Task Description:

A CO₂ laser is used to provide the heat source. The profile of the laser intensity in the radial direction can be a Heaviside function or a Gaussian function with variable beam diameter. The material of the test chamber is a copper water jacket, providing well-controlled wall temperature. The bottom wall of the test cell is insulated. An IR imager is used to measure surface temperature distribution and several thermocouples are implanted in the test chambers, including one at the bottom. Critical powers of the CO₂ laser at the onset point of oscillatory flow are measured at various aspect ratios and dynamic Bond numbers.

Task Significance:

The strategy of this study is to first compare the measured onset conditions for oscillatory flows with results from linear stability analysis. With the designed experimental conditions, surface tension and buoyancy effects are equally important. If close comparison between experimental and numerical results can be obtained, it could support the validity of numerical prediction of the onset conditions for pure Marangoni flow. Results obtained in this study can help the design of surface tension driven convection experiments in space. Furthermore, a deeper understanding of the thermocapillary flow can be achieved, and the knowledge can be used to improve materials processing procedures.

Progress During FY 1996:

The transitions of organized oscillations to chaos in surface-tension-driven convection have been studied. Power spectra of surface temperature at a fixed location were obtained from time history of the data with fast-Fourier-transformation. As opposed to pure Rayleigh convection, no subharmonic modes have been observed in the route to chaos when both thermocapillarity and buoyancy effects are significant. In addition to power spectra, phase trajectories for surface temperature at a fixed location are studied. Various strange attractors have been observed. However, fully chaotic flows occur only in limited number of test cases due to the fast evaporation of silicone oil. A pressurized chamber is necessary to suppress strong evaporation for achieving wide range of test conditions.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	1
PhD Students:	0	PhD Degrees:	0

TASK INITIATION: 10/92 EXPIRATION: 10/95

PROJECT IDENTIFICATION: 962-24-05-67

NASA CONTRACT NO.: NAG3-150

RESPONSIBLE CENTER: LeRC

Light Scattering Studies of Relative Motions of Solid Particles in Turbulent Flows

PRINCIPAL INVESTIGATOR: Prof. Penger Tong

Oklahoma State University

CO-INVESTIGATORS:

Goldburg, W.I.

University of Pittsburg

Task Objective:

The primary objective of this task is to understand the motion of colloidal particles under different random forces when their density is different from the carrier fluid. Particularly, the project entails experimental studies of the particle motion in turbulent flows and in sedimentation, in which hydrodynamic interactions between the small colloidal particles affect the dynamics of the particles at different time and length scales.

Task Description:

A series of light scattering experiments will be carried out to study the particle dispersion phenomena in two well characterized turbulent flows. One is turbulent thermal convection in water and the other is a turbulent grid flow in a water channel. New light scattering technique will be developed to measure the spatial distribution of the particles, the relative velocity of the particle pairs separated by various distances, and fluctuations of the particle settling velocity.

Task Significance:

The proposed research will provide important and reliable for further developing an understanding of the hydrodynamic interactions between the colloidal particles at equilibrium and in turbulent flows. These experiments are of fundamental interest in revealing phenomenology and testing theoretical models, and they are also relevant to studies of other two-phase flows, which have many practical applications. The new light scattering methods to be developed for this project will have a myriad of applications in the discipline of fluid dynamics.

Progress During FY 1996:

The PI has completed the study of the depletion interaction in a mixture of colloid and non-adsorbing polymer. Using the small-angle neutron scattering technique, PI measured the colloidal structure factor $S(q)$, which is directly related to the interaction potential $U(r)$ between the particles. For the first time, the experiment demonstrates that the polymer-induced depletion attraction can be used to accurately describe the colloidal interaction in polymer solutions. The experiment reveals the effectiveness of using polymer to control the colloidal interaction potential $U(r)$. A short paper reporting the main results of this work has been published in Physical Review Letters, and a longer paper with more experimental details is accepted for publication in Physical Review E.

Using the small-angle neutron scattering technique, PI is also studying the adsorption phenomena for the colloidal particles suspended in end-functionalized polymer solutions. The experiment reveals that the presence of adsorbed polymer molecules on the colloidal surfaces greatly reduces the depletion attraction due to the free polymer chains in the solution. This work has been reported in the American Physical Society March meeting at St. Louis, and PI is now preparing a manuscript for publication.

In the third experiment, PI is studying the motion of colloidal particles when they are suspended in a turbulent flow. Dynamic light scattering technique is used to measure the velocity and its statistics for particle pairs separated by a distance l . To overcome the undesired destructive interference effect arisen when the length l is changed in the dynamic light scattering scheme to measure the velocity difference. This method has been successfully tested in the PI's laboratories. This work will be reported in an international conference on Photon Correlation and Scattering at Capri, Italy, and PI is now preparing a manuscript for publication.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/94 EXPIRATION: 8/97

PROJECT IDENTIFICATION: 962-24-05-98

NASA CONTRACT NO.: NAG3-161

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Ye, X., Narayanan T., Tong, P., and Huang, J.S., Neutron scattering study of depletion interactions in a colloid-polymer mixture. Phys. Rev. Lett., 76, 4640 (1996).

Ye, X., Narayanan, T., Tong, P., Huang, J. S., Lin M. Y., Carvalho, B. L., and Fetters, L. J., Depletion interaction in colloid-polymer mixtures. Phys. Rev. E., (accepted, 1996).

Proceedings

Tong, P., "Polymer-induced depletion interaction and its effect on colloidal sedimentation in colloid-polymer mixtures." Proceedings of Third Microgravity Fluid Physics Conference 1996.

Presentations

Goldburg, W. I., "Using homodyne photon correlation spectroscopy to measure velocity differences over varying length scales." Photon Correlation and Scattering Topical Meeting and Tabletop Exhibit, Capri, Italy, August 21-24, 1996.

Narayanan, T., Ye, X., Tong, P., and Huang, J.S., "A neutron scattering study of depletion interactions in a colloid-polymer mixture." American Physical Society March Meeting, St. Louis, March 18-22, 1996.

Tong, P., "Polymer-induced depletion interaction and its effect on colloidal sedimentation in colloid-polymer mixtures." Third Microgravity Fluid Physics Conference, Cleveland, Ohio June 13-15, 1996.

Tong, P., "Neutron scattering studies of interactions in mixtures of colloid and polymer." Physics Department Colloquium, University of North Texas, April 16, 1996.

Tong, P., Ye, X., and Huang, J. S., "Adsorption of end-functionalized polymer molecules on colloidal spheres." American Physical Society March Meeting, St. Louis, Missouri, March 18-22, 1996.

Studies of Particle Sedimentation by Novel Scattering Techniques

PRINCIPAL INVESTIGATOR: Prof. Penger Tong

Oklahoma State University

CO-INVESTIGATORS:

Ackerson, B.J.

Oklahoma State University

Task Objective:

The objectives of this task are: (1) develop a robust and compact velocimeter system suitable for incorporation into existing NASA flight apparatus, and (2) use the new dynamic light scattering technique on the ground to study sedimentation phenomena of small colloidal particles.

Task Description:

The project consists of two parts. The first deals with the development of a new velocimeter system useful for future NASA flight experiments. A two-color cross-correlation spectroscopy has been developed by the PI's and has demonstrated with the capability of accurately measuring the local velocity and its statistics. The proposed research will refine the instrument further to permit multi-point, two-component velocity measurements and to reduce the measuring time. Diode lasers and fiber optics will be used to reduce the size of the instrument and thereby create a robust and compact velocimeter suitable for incorporation into existing NASA flight apparatus.

The second part of the project involves a series of light scattering experiments to study velocity fluctuations and spatial correlations in dispersions of colloidal spheres settling at low Peclet number as a function of the particle volume fraction and interaction potential. In addition, scattering measurements will be carried out to study the rotation of optically and gravitationally anisotropic particles.

Task Significance:

The development of a small and robust velocimeter will provide a new tool to measure the flow velocity and its statistics, which is useful in the general area of the microgravity fluid physics. The new instrument will also have a myriad of applications in the discipline of fluid dynamics. The proposed light scattering experiments will provide an important and reliable body of data for further developing an understanding of hydrodynamic interactions in the sedimentation of small colloidal particles.

These experiments are of fundamental interest in revealing phenomenology and testing theoretical models, and they are also relevant to many practical applications ranging from dewatering of coal slurries and processing of drilling and mining fluids containing rock and mineral particles to various laboratory techniques for separating and analyzing colloidal particles and biological macromolecules.

Progress During FY 1996:

A new experiment has been initiated to study the sedimentation of heavy colloidal particles in a polymer solution. A key parameter in controlling the settling of the particles is their interaction potential $U(r)$. Our recent neutron scattering measurements (supported by another NASA grant) have shown that adding polymer molecules into a colloidal suspension is an effective way to control the potential $U(r)$. With the well characterized colloid-polymer mixture, we are now investigating how the colloidal particles settle in the polymer solution and how the polymer-induced depletion interaction affects the particle settling velocity.

It is found that when the colloid concentration is low, the particle interaction can be ignored and individual particles experience an increasing viscosity with the addition of the polymer molecules. For high colloid concentrations, however, the polymer-induced depletion attraction overcomes the increase in viscosity, and the particle settling velocity is increased considerably. This is a remarkable effect and we are now analyzing the data and prepare a manuscript for publication. Preliminary results have been reported in the Third Microgravity Fluid Physics Conference at Cleveland, Ohio. Because the basic molecular interactions in our colloid-polymer mixture are tuned to be simple, the experiment can be used to critically examine the current theory for colloidal sedimentation. Once this is understood, a simple sedimentation method can be developed to probe the interactions in the colloidal suspensions.

The project of developing a small velocimetry system started in the Summer of 1996. Necessary paper work has been done to purchase a diode laser system, a dual-photomultiplier detecting system, and other fiber-optical components needed to build the velocimeter. A new graduate student will start to work on the project in the Fall of 1996.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-185

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Tong, P., "Polymer-induced depletion interaction and its effect on colloidal sedimentation in colloid-polymer mixtures." Proceedings of Third Microgravity Fluid Physics Conference, NASA Conference Publication 3338, 413-418, July 13-15, 1996.

Presentations

Tong, P., "Polymer-induced depletion interaction and its effect on colloidal sedimentation in colloid-polymer mixtures." Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 13-15, 1996.

Tong, P., "Velocity measurements in turbulent Thermal convection using lasers." Laser and Photonics Research Seminar, Laser Center, Oklahoma State University, August 8, 1996.

Tong, P., "Interactions in mixtures of colloid and polymer." Workshop on Complex Fluids, China Center of Advanced Science and Technology, Beijing, China, September 23-28, 1996.

Acoustic Streaming in Microgravity: Flow Stability and Heat Transfer Enhancement

PRINCIPAL INVESTIGATOR: Dr. Eugene H. Trinh

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Gopinath, A.
Sadhal, S.S.Naval Post-Graduate School
University of Southern California

Task Objective:

- a. Experimental flow field mapping for isothermal streaming around a levitated sphere in a gas environment. Full field visualization studies and streaming velocity measurements will be carried out for streaming Reynolds number $Rs < 50$.
- b. Experimental development and implementation of liquid cell streaming flow studies. The initial approach will be based on an existing 22 kHz ultrasonic resonant cell previously developed for liquid-liquid drop dynamics studies.
- c. Initial analysis will be performed for the isothermal streaming around a sphere superposed on a steady axisymmetric convective flow. The derivation of the isothermal flow field configurations and the stability analysis will be initiated.

Task Description:

A second order effect associated with high intensity sound field, acoustic streaming has been historically investigated to gain a fundamental understanding of its controlling mechanisms and to apply it to practical aspects of heat and mass transfer enhancement. The objectives of this new research project are to utilize a unique experimental technique implementing ultrasonic standing waves in closed cavities to study the details of the generation of the steady-state convective streaming flows and of their interaction with the boundary of ultrasonically levitated near-spherical solid objects. The goals are to further extend the existing theoretical studies of streaming flows and sample interactions to higher streaming Reynolds number values, for larger sample size relative to the wavelength, and for a Prandtl and Nusselt numbers parameter range characteristic of both gaseous and liquid host media. Experimental studies will be conducted in support to the theoretical developments, and the crucial impact of microgravity will be to allow the neglect of natural thermal buoyancy. The direct application to heat and mass transfer in the absence of gravity will be emphasized in order to investigate a space-based experiment, but both existing and novel ground-based scientific and technological relevance will also be pursued.

Task Significance:

The active control of the rates of heat and mass transfer in non-isothermal systems is often a desired capability associated with many industrial and technological practices. In general, this is accomplished by varying the interfacial area and by inducing appropriate flow fields in the medium through which transport takes place. For example, the control of gas and melt flow rates, atomizing gas pressure, initial melt temperature, and host medium conductivity are used to change the quenching rate in gas atomization processes of powder metallurgy. In the case of multi-component or multi-phase disperse systems dealing with direct contact heat transfer, distillation, or liquid extraction, some enhancement of transport or reaction rates has been obtained through the use of electric fields which induce drop oscillations as well as internal flow within the fluid particle. Thus, even for Earth-bound activities for which natural convection is often important, the control of flow fields in the vicinity of the contact interfaces is of significant practical value.

In a low gravity environment, the drastic reduction of natural buoyancy will make the contribution from any externally imposed flow field even more important. For example, heat transfer processes involving change of phase (such as boiling) are drastically affected by the elimination of buoyancy-driven removal of vapor bubbles. In the absence of artificially induced flows, heat or mass transfer in microgravity is expected to be dominated by radiation, conduction, or diffusion processes. A minor contribution may also come from thermocapillary flows (Marangoni convection) in the case of free liquid-gas interfaces. In currently utilized manned spacecraft, however, another source of steady-state or time-varying convective flows arises from the residual fluctuating acceleration background (the

so-called "g-jitters"). The appearance of steady-state flows have been predicted, and under certain conditions involving a range of values for the Prandtl number, the vibration frequency, and for a large enough Rayleigh number, these flows could significantly impact heat transport processes.

Acoustic streaming-induced convective flows have also been shown to substantially enhance heat and mass transfer, even under the full action of the Earth gravitational field. A detailed understanding of this effect is not yet available, however, because natural convection interferes with accurate heat and mass transport measurements under most experimental conditions found in Earth-based laboratories. The exception might be found at very high acoustic pressure at which stage the second order streaming flow becomes turbulent and theoretical analysis is even more complicated. We plan to carry out a ground-based research program to experimentally and theoretically examine both the configuration and stability of acoustically induced streaming flows in order to advance the understanding of the physical mechanisms responsible for their generation, and to develop a predictive model for the observed enhancement in the rates of heat and mass exchange. The capability to virtually eliminate steady natural convection in microgravity will be examined to assess the possibility of performing experimental measurements that are not possible on Earth, but that could impact the understanding of both Earth-based and microgravity problems. We thus believe that the problem of controlling heat and mass transfer through induced external flow is important to technological applications both on Earth and in microgravity, that acoustic streaming-modulated transport processes are of current scientific interest, and that this phenomenon could be better understood by carrying out microgravity studies. Further, we think that the similarity between acoustically and g-jitters-induced streaming is significant enough to be useful in the investigation of the microgravity streaming problem.

Progress During FY 1996:

The research task has been officially initiated on 8/01/96 with the establishment of a JPL account.

We are in the process of adding a post-doctoral fellow to this research effort, and we anticipate that will be completed by December 1996.

A new laboratory apparatus is being designed to integrate thermal control and optical flow visualization from suspended particles. The first task planned is to quantitatively characterize the streaming flow fields in a closed isothermal cubical cavity with a standing wave at 23 kHz. The influence of the specific design of the ultrasonic driver and reflector and of the cavity wall material will be of particular interest since it appears that they influence both the symmetry and stability of the flow fields. Streaming flows will be investigated using both liquid as well as gas host media.

As a first preliminary investigation, qualitative flow visualization of flow inside a trapped air bubble in a liquid-filled ultrasonic cavity has been obtained. The results indicate measurable air motion in the inside the ultrasonically trapped bubble, but more importantly, indicates that the dynamics of the gas-liquid interface are greatly perturbed by the induction of capillary waves at the bubble surface. These were the first ever recorded flows within a gas bubble trapped in 1 G. The implications of streaming flows on the transport dynamics at the bubbles gas-liquid interfaces have not been determined yet, but they impact the fundamental physical phenomena affecting single bubble sonoluminescence.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 8/96 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 962-24-00

RESPONSIBLE CENTER: LeRC

Computational Studies of Drop Collision and Coalescence

PRINCIPAL INVESTIGATOR: Prof. Grétar Tryggvason

University of Michigan

CO-INVESTIGATORS:

Jacqmin, D.

NASA Lewis Research Center (LeRC)

Task Objective:

The objective of this research is to investigate the behavior of bubbles and drops in microgravity by full numerical solutions of the governing equations. The collision and thermal migration of drops are studied in detail to provide essential input for material processing and fluid handling in space. These problems also serve as a test bed for refinements and extensions of the numerical technique being used, thus helping to develop the capability to predict accurately the behavior of free-surface fluid systems.

Task Description:

A numerical technique, based on explicit tracking of the interface between two immiscible fluids, is used in this study. This method has now been extended to deal with both the thermal migration and the rupturing of thin films.

Task Significance:

The unique aspect of the method is that it accounts fully for both inertia and viscous effects in both fluids and allows the inclusion of surface tension. It is also well suited for complicated interface geometries and has been implemented for fully three-dimensional flows. The basic aspect of this method is described in the *Journal of Computational Physics*, vol. 100 (1992), p. 25.

Progress During FY 1996:

Our research is aimed at developing a basic understanding of the behavior of drops in microgravity and developing numerical tools to allow accurate predictions of their behavior. We have focused on: Collision of drops, thermal migration of both bubbles and drops, and the motion of drops in shear flows.

Most of our work has been done using explicit tracking of the boundaries between fluids. We have simulated the head-on collision of two equal size drops for a wide range of Weber and Reynolds numbers. We have also looked at off-axis collisions. Simulations have been compared in detail to experiments and there is good agreement. We have examined in detail the evolution of drops in shear and pressure-driven flow between stationary walls. Both the fluidization of a layer of drops initially near a wall as well as the long time evolution of an initially uniform distribution of drops has been examined. We have carried out simulations of thermal migration of drops focused on the collective behavior of many drops as they migrate through a channel toward a hot surface. These show that there is a strong tendency of the drops to congregate and to form layers across the channel.

We have also been developing continuum surface tension methods for two-phase flow, particularly phase field methods that are conservative of energy and momentum. These have been used to study annular flow breakup and drop formation caused by capillary instabilities, contact line flows, and drop breakup and re-coalescence in oscillating flows.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	3	PhD Degrees:	3

TASK INITIATION: 1/92 EXPIRATION: 10/95

PROJECT IDENTIFICATION: 963-24-05-07

NASA CONTRACT NO.: NAG3-131

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Nobari, M.R.H. and Tryggvason, G., Numerical simulations of three-dimensional drop collisions. *AIAA Journal*, 34, pp. 750-755 (1996).

Nobari, M.R., Jan, Y.-J., and Tryggvason, G., Head-on collision of drops--a numerical investigation. Phys. Fluids, 8, pp. 29-42 (1996).

Proceedings

Jacqmin, D., "An energy approach to the continuum surface tension method: application to droplet coalescences and droplet/wall interactions." Proceedings of the 1995 ASME IMECE, November 1995.

Presentations

Jacqmin, D., "An energy approach to the continuum surface tension method." AIAA 96-0858, AIAA 34th Aerospace Sciences Meeting and Exhibit, 1996.

Nonlinear Bubble Interactions in Acoustic Pressure Fields

PRINCIPAL INVESTIGATOR: Prof. John Tsamopoulos

State University of New York, Buffalo

CO-INVESTIGATORS:

Ashgriz, N.

State University of New York, Buffalo

Task Objective:

This project proposes both theoretical and experimental studies of the interactions between bubbles immersed in an immiscible liquid. Specific objectives include the following:

1. To investigate the conditions when linearly accelerating motion of two interacting bubbles turn into a spiral motion of one of them.
2. To study the delay and prevention of break up of accelerating bubbles.
3. To incorporate bubble velocity and fluid viscosity into a coalescence model.
4. To study the coalescence of two bubbles.

Task Description:

The analytical study will focus on bubble oscillations and interactions of moderately large amplitude and will determine conditions under which the axisymmetric flow turns into three-dimensional. For viscous liquids or large deformation either the Boundary Element method or a combination of Finite Elements with the Volume of Fluid method will be used. Bubbles will be suspended in an immiscible liquid using the acoustic levitation technique for the experimental part of this project. Bubble motions and interactions will be induced by an additional acoustic field. The bubble motions, shape oscillations, collision and breakup will be recorded with high-speed cinematography.

Task Significance:

The results from this project will be beneficial to others in the bubble dynamics studies. It is well known that the formation and collapse of cavities of gas inside a flow stream cause erosion in fluid-handling equipment. The effect of a properly tuned acoustic field may help in the correct detection of submerged objects in the production of bubble dispersions.

Progress During FY 1996:

During this reporting period, the following have been accomplished:

1. Experiments continued to be performed with bubbles of various sizes and the following modes of interaction were identified:

a) Pairs of bubbles of 0.5-2 mm radius, larger than the resonance size of 0.12 mm at the applied frequency of 22.5 kHz, showed attraction forces of interaction; their motion is finalized with collisions;

b) Pairs of bubbles around 0.12 mm did not collide, they exhibited oscillatory behavior: attraction when the distance between them is large comparatively to their radii, repulsion for small separations, equilibrium at rest for certain distances;

c) Small bubbles showed same type of behavior nearby large bubbles: attraction followed by steep repulsion when they approached under some critical distance.

d) Systems consisting of more than two bubbles were observed with a regular video camera in order to have accurate enough images; one experiment featured two bubbles larger than the resonance radius, attracting each other, but prevented from colliding by two smaller bubbles in between them.

2. The experiments were explained with an analytic mathematical model allowing parametric studies for the system of two interacting bubbles. The interaction between the two bubbles is then replaced by a force field with a new formula, different from the previous theoretical approaches.

The expression for the secondary Bjerknes forces has a term proportional to R^{-2} which can be either an attraction or a repulsion (depending mainly on the values of the phase shifts), and a term proportional to r^{-5} , always a repulsion. This new type of dependence upon the mutual distance r enabled the analytic model to explain all the patterns of interactions observed during the experiments.

3. In the case of two equal bubbles, the dynamical system formed by the two equations of motion (nonlinear ordinary second order differential equations) reduces to only one ODE for the relative distance. This particular case is then analyzed in new time and space variables, which allow to identify two important dimensionless parameters.

An exact analytic solution for the equation can be obtained using elliptic integrals and their inverse functions; also, simpler, approximate solutions are obtained for various magnitudes of the energy level.

For $q < 0.943$ (bubbles smaller than the resonance size) it is shown that the net effect of the force field given by (1) is a repulsion at any distance between the two bubbles; for $q > 0.970$ the net effect is an attraction at all physically possible distances between the bubbles; for $0.943 < q < 0.970$ (bubbles comparable with the resonance size) the force field shows an equilibrium point, with the effect changing from attraction at large distances to repulsion at small distances and thus oscillations of the system can occur, depending on the initial conditions (i.e. the energy level).

The results of the analytical approach were verified by the numerical solution of the equations of motion.

4. The analytic method from above was extended to the more general case of two unequal bubbles. Their motion was decomposed in a relative motion, characterized by the same ODE as the system of two equal bubbles, and a motion of the center of mass of the combined system. General analytic relations were developed and the limiting cases (equal bubbles) and (large size difference) were verified with them. The conclusions explained consistently the experiments described in 1c and d. Future work is needed to continue the analysis in the following directions: - find the parameters and the patterns of the motion of the center of mass of the system of two unequal bubbles; - find what is the effect of a dissipative perturbation (i.e. drag forces) on these conservative systems; - study the dynamics of systems consisting of three or more bubbles interacting through this force field, extending the results to populations of bubbles subject to acoustic fields.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 2

TASK INITIATION: 6/94 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-24-05-99

NASA CONTRACT NO.: NAG3-162

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Barbat, T., Ashgriz, N., and Lie, C., Interaction between gas bubbles in acoustic pressure fields. *Journal of Fluid Mechanics*, (1996).

Presentations

Ashgriz, N., "Dancing bubbles." Department of Mechanical Engineering, University of Victoria, Victoria, CANADA, May 15, 1996.

Ashgriz, N., "Dancing bubbles." Department of Mechanical Engineering, The University of British Columbia, Vancouver, CANADA, May 16, 1996.

Ashgriz, N., "Dancing bubbles." Department of Physics, State University of New York at Buffalo, Buffalo, NY, September 10, 1996.

Barbat, T., Ashgriz, N., "Dancing bubbles and drops." 9th Annual Conference on Liquid Atomization and Spray Systems, San Francisco, CA, May 19-22, 1996.

Barbat, T., Ashgriz, N., and Liu, C.S., "Dynamics of two interactive bubbles in an acoustic field - part I: theory." Annual Meeting of the Division of Fluid Dynamics of American Physical Society, Syracuse, New York, November 20-22, 1996.

Barbat, T., Ashgriz, N., and Liu, C.S., "Dynamics of two interactive bubbles in an acoustic field - part II: experiments." Annual Meeting of the Division of Fluid Dynamics of American Physical Society, Syracuse, New York, November 20-22, 1996.

Barbat, T., Ashgriz, N., Liu, C.S., "Nonlinear bubble interactions in acoustic pressure fields." Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 13-15, 1996.

Residual Accelerations in a Microgravity Environment

PRINCIPAL INVESTIGATOR: Prof. Jorge Viñals

Florida State University

CO-INVESTIGATORS:

Sekerka, R.F.

Carnegie-Mellon University

Duval, W.

NASA Lewis Research Center (LeRC)

Task Objective:

This research program aims at developing a realistic theoretical model of the high frequency components of the residual acceleration field (or g-jitter) on-board spacecraft, and at studying its effect on a variety of typical fluid experiments.

Task Description:

The high-frequency components of the residual acceleration field on board Space Shuttle are modeled as a stochastic or random process; that is, as a succession of random values of the intensity and orientation of the acceleration. Our research is divided into two major parts, one analytic and the other numerical in character. In the first part, we formulate a hydrodynamic problem that explicitly includes a random, time-dependent gravitational acceleration which is modeled as a narrow band noise. In the second part, we develop numerical algorithms to simulate this type of random field and incorporate them into Navier-Stokes equation solvers.

Task Significance:

All space experiments performed in a manned space environment are exposed to high frequency residual accelerations (g-jitter). Such an environment can significantly affect experimental results. A combined analytic and numerical approach has been undertaken to determine what regimes of g-jitter could affect experiments conducted in a microgravity environment. A generic class of problems has been considered with emphasis on fluid physics and materials science experiments.

Progress During FY 1996:

We have addressed the motion of a particle suspended in an incompressible fluid of different density, when the fluid is subjected to an effective acceleration field like the one described above. This type of motion has been termed inertial random walk because of the similarity with Brownian motion. The asymptotic mean squared velocity of a particle subjected to narrow band noise was determined analytically.

The particle undergoes diffusive motion (the mean squared displacement is proportional to time), with an effective diffusion coefficient that is proportional to the intensity of the fluctuating acceleration. Therefore, from a measure of the appropriate autocorrelation function, it should be possible in principle to determine independently the parameters that define g-jitter. Knowledge of this sort could conceivably lead to the construction of an instrument that would complement the data set provided by accelerometers.

This result is further significant because it is more generally valid for situations in which the response of the system can be described by a single mode that responds additively to the forcing. In that case, the equation above illustrates how the parameters of the jitter modify earlier results used to define tolerable levels of residual accelerations as a function of the frequency of the disturbance. If the correlation time of the noise is sufficiently large compared to the friction coefficient of the mode in question, the equation reduces to the classical result. Otherwise (and most notably in the limit of white noise the amplitude of fluctuation becomes independent of frequency.

Second, progress has been made in connection with coarsening experiments to be conducted in microgravity in the near future. A residual acceleration field can produce a number of deleterious effects on otherwise purely diffusive controlled coarsening. We have focussed on two such effects: random motion of the suspended particles induced by the effective (random) buoyant force and the concomitant increase in the likelihood of particle coalescence, and additional flow in the fluid phase caused by g-jitter and its effect on solute mass transport. Numerical estimates have

been obtained for a solid-liquid mixture of Sn-rich particles in a Pb-Sn eutectic liquid, the system that will be used in a forthcoming microgravity experiment (CSLM, P. Voorhees, PI). We have found that, for the conditions and duration of the experiment, the average square displacement induced by the white noise component of the residual acceleration field is much larger than that induced by the monochromatic component, but it is still about one half of the expected average particle size at the end of the coarsening experiment. Therefore Brownian motion induced by g-jitter will not lead to appreciable motion of the precipitate particles relative to their size.

Estimating the effect of g-jitter on mass transport in the fluid phase is far more complex. In the limit of Stokes flow and interacting solid particles through a mean field approximation, (the former is appropriate for the size of the coarsening particles involved), g-jitter induced flow acts to renormalize the solute diffusivity. Again, we have found that for the parameters appropriate for the experiment, this change is negligible.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0 BS Degrees: 0
 MS Students: 0 MS Degrees: 0
 PhD Students: 2 PhD Degrees: 1

TASK INITIATION: 6/91 **EXPIRATION:** 3/96

PROJECT IDENTIFICATION: 962-24-05-36

NASA CONTRACT NO.: NAG3-129

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:
Journals

Gurtin, M., Polignone, D., and Vinals, J., Two-phase binary fluids and immiscible fluids described by an order parameter. *Mathematical Models and Methods in Applied Sciences*, (in press).

Thomson, J.R. and Vinals, J., Statistical saturation of buoyant flow induced by a fluctuating acceleration. *AIAA J.*, vol. 34, pp. 975 (1996).

Zhang, W. and Vinals, J., Square patterns and quasi-patterns in Faraday waves in low viscosity fluids. *Phys. Rev. E*, vol. 53, R4283, (1996).

Zhang, W. and Vinals, J., Pattern formation in weakly damped Faraday waves. *J. Fluid Mech.*, (in press).

Presentations

Thompson, J.R., Drolet, F., and Vinals, J., "Fluid physics in a fluctuating acceleration environment." *Proceedings of the Third Microgravity Fluid Physics Conference*, Cleveland, OH, June 1996.

Fluid Physics in a Stochastic Acceleration Environment

PRINCIPAL INVESTIGATOR: Prof. Jorge Viñals

Florida State University

CO-INVESTIGATORS:

Sekerka, R.

Carnegie-Mellon University

Duval, W.

NASA Lewis Research Center (LeRC)

Task Objective:

This research program aims at developing a realistic theoretical model of the high frequency components of the residual acceleration field (or g-jitter) on board spacecraft, and at studying its effect on a variety of typical fluid experiments.

Task Description:

The high-frequency components of the residual acceleration field on board Space Shuttle are modeled as a stochastic or random process; that is, as a succession of random values of the intensity and orientation of the acceleration. Our research is divided into two major parts, one analytic and the other numerical in character. In the first part, we formulate a hydrodynamic problem that explicitly includes a random, time-dependent gravitational acceleration which is modeled as a narrow band noise. In the second part, we develop numerical algorithms to simulate this type of random field and incorporate them into Navier-Stokes equation solvers.

Task Significance:

All space experiments performed in a manned space environment are exposed to high frequency residual accelerations (g-jitter). Such an environment can significantly affect experimental results. A combined analytic and numerical approach has been undertaken to determine what regimes of g-jitter could affect experiments conducted in a microgravity environment. A generic class of problems has been considered with emphasis on fluid physics and materials science experiments.

Progress During FY 1996:

Ideal bifurcations can occur in model systems that are described by ordinary differential equations when some of the parameters of the model are varied. At the bifurcation point, the nature of the stationary solutions of the differential equations changes in a qualitative way. When noise is added, a number of different phenomena may be observed, including a shift of the bifurcation point, a smearing" of the bifurcation point into a region of finite width, or a change in the nature of the bifurcation. Little can be said in general because of the relative latitude in the choice of the noise for a particular system, and the mathematical difficulty associated with analytical solutions.

We have started work on the effect of noise in general, and narrow band noise in particular, on an oscillatory or Hopf bifurcation. Special attention will be paid to possible resonance effects between the Hopf frequency at the bifurcation and the frequency of the driving force, the relative stability of traveling or standing wave solutions, shifts in the stability boundaries, and the behavior close to a co-dimension two point in the case of a system externally driven. Oscillatory instabilities are important in a number of areas of microgravity research, especially in connection with crystal. In this case, the existence of temperature and composition gradients in the melt can result in buoyancy driven convection, even at the reduced gravity levels of space. In multicomponent fluids, the onset of convection is oscillatory when the separation ratio is negative; i.e., when the temperature field is destabilizing whereas the composition field is stabilizing.

We are initially focusing on the shift of the onset of instability when the system is driven by noise, and the underlying set of equations describes a Hopf bifurcation in the absence of noise.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	1
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 6/96 **EXPIRATION:** 6/00

PROJECT IDENTIFICATION: 962-24-00

NASA CONTRACT NO.: NAG3-188

RESPONSIBLE CENTER: LeRC

Experimental Study of the Vapor Bubble Thermosyphon

PRINCIPAL INVESTIGATOR: Prof. Peter C. Wayner, Jr.

Rensselaer Polytechnic Institute

CO-INVESTIGATORS:

Plawsky, J.

Rensselaer Polytechnic Institute

Task Objective:

The objective of this effort is to better understand the physics of evaporation and condensation as they affect the heat transfer processes in a vapor bubble thermosyphon (VBT). In small systems, interfacial intermolecular forces can be used to control fluid flow and heat transfer. The VBT, one such system, consists of a small enclosed container partially filled with a liquid. When a temperature difference is applied to the ends of the VBT, evaporation occurs at the hot end and condensation at the cold end -- resulting in a very effective heat transfer device. The research performed under this ground-based study has led to a NASA supported definition-phase flight experiment.

Task Description:

A transparent VBT will be designed and developed. The microscopic intermolecular force (pressure) field, which is a function of the liquid thickness profile, will be measured using microcomputer enhanced video microscopy based on interferometry. The temperature field will be measured using the interline absorbed film thickness and small temperature sensors.

Models of the transport processes in the contact line region of a VBT which include the effects of liquid-solid and liquid-vapor intermolecular forces have already been developed. As part of this effort these models will be further refined and the transport characteristics of VBTs will be obtained by comparing the experimental data to numerical solutions of the model.

Task Significance:

By studying liquid-film thicknesses and temperatures in VBT, a better understanding of the processes can be gained that will lead to optimization of VBT designs.

Progress During FY 1996:

The experimental and theoretical studies were divided into equilibrium and non equilibrium studies of the CVBT. We note that we changed the name of the experimental design from VBT to CVBT (Constrained Vapor Bubble Thermosyphon) which is more descriptive.

The following conclusions are based on the *equilibrium* studies:

1. The use of an image analyzing interferometer, IAI, with a constrained vapor bubble thermosyphon, CVBT, was demonstrated under equilibrium conditions at 1g.
2. Using the augmented Young-Laplace equation, good agreement between the theoretical and experimental values of the dispersion constant was obtained.
3. A gravitational field restricts the range of forces that can be studied because the curvature gradient, K' , is a function of gravity.
4. The ground based studies demonstrated that a "relatively simple" flight experiment can be designed to evaluate the augmented Young-Laplace equation using the CVBT under equilibrium conditions.

A flight experiment to study the augmented *equilibrium* Young-Laplace equation is warranted.

The following conclusions are based on the *non equilibrium* studies:

1. Experimental and theoretical techniques to study non isothermal transport processes in the constrained vapor bubble thermosyphon (CVBT) were developed.
2. The transport processes can be evaluated by measuring the liquid film profile using an image-analyzing interferometer, which gives the pressure field and the temperature field.
3. Thermoelectric coolers can be used to control the temperature level in the condensation region and, therefore, the length of the approximately "adiabatic" surface region.

4. For an accurate study, it is important to *control* both the input power and the outside surface heat flux distribution.
5. High values for the axial thermal conductance in the "adiabatic" surface region were demonstrated.
6. A microgravity flight experiment under non equilibrium conditions is warranted. However, additional development work for the non isothermal system is required.

We also performed equilibrium studies using water. Water is obviously a very complex fluid to study experimentally when interfacial forces are being emphasized. However, the use of the CVBT experimental cell will add new and significant information concerning the water/glass system. In addition, a well controlled water heat exchanger would be highly desirable for the microgravity environment. Some of these results are described in our 1995 presentation paper for the Annual Meeting of AIChE. This work is also continued under a separate NSF grant.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	1
PhD Students:	2	PhD Degrees:	0

TASK INITIATION: 12/92 EXPIRATION: 11/95

PROJECT IDENTIFICATION: 962-24-05-44

NASA CONTRACT No.: NAG3-139

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Karthikeyan, M., Huang, J., Plawsky, J., and Wayner, P.C., Jr., "Initial nonisothermal experimental study of the constrained vapor bubble thermosyphon." Proceedings of the ASME 31st National Heat Transfer Conference (vol. 5) pp 121-129, ASME, NY, NY, 1996.

Presentations

Karthikeyan, M., Huang, J., Plawsky, J., and Wayner, P.C., Jr., "Initial nonisothermal experimental study of the constrained vapor bubble thermosyphon." Paper presented at the National Heat Transfer Conference, Houston, TX, August 3-6, 1996.

Karthikeyan, M., Huang, J., Plawsky, J.L., and Wayner, P.C., Jr., "Experimental study of the constrained vapor bubble thermosyphon." Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 13-15, 1996.

Reyes, R., and Wayner, P.C., Jr. "Thin film profile of an extended meniscus in a glass cuvette." Material concerning water presented at the 1995 Annual Meeting of A.I.Ch.E., Miami Beach, FL, November 15-18, 1995.

Study of Two Phase Flow Dynamics and Heat Transfer at Reduced Gravity

PRINCIPAL INVESTIGATOR: Prof. Larry Witte

University of Houston

CO-INVESTIGATORS:

McQuillen, J.B.

NASA Lewis Research Center (LeRC)

Task Objective:

The objective of this study is to develop and experimentally verify theoretical models that predict gas-liquid flow regimes and their characteristics in reduced gravity.

Task Description:

Reduced-gravity experiments were conducted in NASA aircraft to measure the previously listed two-phase flow parameters for a range of tube diameters, gas and liquid flow rates, and fluid properties. The gas phase for the experiments was air; the liquids employed were water, water-glycerin mixtures, and water-zonyl mixtures. A theoretical modeling effort was integrated with the experimental efforts.

Task Significance:

The purpose of this study is to achieve a better understanding-better predictability-of two-phase (gas-liquid) flow in pipes to assist in the design of space-based power and thermal management systems and of the terrestrial-based nuclear power plants and oil and natural gas pipelines.

Progress During FY 1996:

The grant expired during 1995 and a closeout procedures were initiated and completed. Several publications and presentations have occurred since the grant closeout.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 12/92 EXPIRATION: 11/94

PROJECT IDENTIFICATION: 963-24-0A-35

NASA CONTRACT NO.: NAG3-510

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Bousman, W.S., Witte, L.C. and McQuillen, J.B. Gas-liquid flow patterns in microgravity: effects of tube diameter, liquid viscosity and surface tension". International Journal of Multiphase Flow, (in press, 1996).

Colin, C., Fabre, J., and McQuillen, J., Bubble and slug flow at microgravity conditions: state of knowledge and open questions. Chemical Engineering Communications, vols 141-142, pp. 155-173 (October 1995).

Fore, L.B., Witte, L.C. and McQuillen, J.B., Heat transfer to annular gas-liquid mixtures at reduced gravity. Journal of Thermophysics and Heat Transfer, vol. 10, no. 4, 633-39 (1996).

Fore, L.B., Witte, L.C. and McQuillen, J.B., Thermal hydraulics of two phase slug flow under reduced gravity. Int. Journal of Multiphase Flow, (accepted, 1996).

Presentations

Fore, L.B. and Witte, L.C., "Two-phase heat transfer in microgravity." invited paper, International Conference on Heat Transfer with Change of Phase, Kielce, Poland, December, 1996.

Fore, L.B., Bousman, W.S. and Witte, L.C. "Two-phase flow dynamics and heat transfer in microgravity." presented at the Energy Week Conference and Exhibit, Houston, TX, January 1996.

Fore, L.B., Witte, L.C. and McQuillen, J.B., "Microgravity heat transfer and pressure drop in gas-liquid mixtures: slug and annular flow." presented at the National Heat Transfer Conference, Houston, TX, 1996.

Witte, L.C., "Fluid dynamics and heat transfer in falling films." Texas A&M University, October 9, 1995.

Witte, L.C., Bousman, W.C., and Fore, L.B., "Studies of two-phase flow dynamics and heat transfer at reduced gravity conditions." NASA Contractor Report 198459, February 1996.

Interactions Between Solidification and Compositional Convection in Alloys

PRINCIPAL INVESTIGATOR: Prof. M. G. Worster

Northwestern University

CO-INVESTIGATORS:

Davis, S.H.

Northwestern University

Task Objective:

The project aims to quantify the effects of convection on the structure and composition of cast alloys. Particular attention is to be focused on the form and influence of convective flows through the interstices of mushy layers during solidification.

Task Description:

Combined experimental and theoretical studies will be undertaken. The laboratory experiments will involve the solidification of aqueous salt solutions, as representatives of general binary systems. The theoretical studies will employ linear and nonlinear stability theory, asymptotic and numerical methods in the development and analysis of predictive mathematical models.

Task Significance:

This study of fluid dynamics during solidification will aid the design of improved casting procedures (e.g., for the manufacture of high-performance turbine blades). It will also improve our understanding of air-sea interactions in polar regions, where the formation of sea ice is a dominant contributor to the global heat budget, leading to better climate modelling a prediction.

Progress During FY 1996:

A new oscillatory mode of convection in mushy layers that we discovered has been analyzed in detail, which has elucidated important interactions between convection and solidification that had not previously been comprehended. Extensive laboratory experiments have been performed to study the formation and evolution of sea ice. The data from these experiments is being used to guide the development of predictive mathematical models that will aid the remote sensing by satellite of the freezing of the arctic oceans, which have a major effect on the changing global climate. A numerical study of convection through chimneys in mushy layers has been undertaken, which has revealed for the first time the detailed structure of the flow and the solute fluxes out of a mushy layer as a function of the external parameters. These results allow the prediction of large-scale segregation of the components of an alloy during casting. A study of melting in layers a few tens of molecular diameters thick is leading to an understanding of the transport of material in partially-molten systems, such as frozen ground and sintered materials. Such transport can far exceed any gravitational flow and is responsible for a number of defects in materials grown in micro gravity.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	3	PhD Degrees:	1

TASK INITIATION: 1/93 **EXPIRATION:** 12/95

PROJECT IDENTIFICATION: 962-24-05-63

NASA CONTRACT NO.: NAG3-140

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Anderson, D.M. and Worster, M.G., Weakly-nonlinear analysis of convection in a mushy layer during the solidification of alloys. *Journal of Fluid Mechanics*, 302, 307-331 (October 1995).

Anderson, D.M. and Worster, M.G., A new oscillatory instability in a mushy layer during the solidification of binary alloys. *Journal of Fluid Mechanics*, 307, 245-267 (1996).

Anderson, D.M., Worster, M.G., and Davis, S.H., Dynamic contact angles in containerless solidification. *Journal of Crystal Growth*, 163/3, 329-338 (1996).

Chiareli, A.O.P. and Worster, M.G., Flow focusing instability in a solidifying mushy layer. *Journal of Fluid Mechanics*, 297, 293-305 (October 1995).

Wettlaufer, J.S., Worster, M.G., Wilen, L.A., and Dash, J.G., A theory of premelting dynamics for all power law forces. *Phys. Rev. Lett.* 76, 3602, (1996).

Nucleation and Chiral Symmetry Breaking under Hydrodynamic Flows

PRINCIPAL INVESTIGATOR: Dr. Xiao-lun Wu

University of Pittsburgh

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The aim of this research is to investigate nucleation and chiral symmetry breaking under shear flow. It has been proposed that the symmetry breaking is a result of a strong first order phase transition coupled to a macroscopic, velocity field. The process, often referred to as autocatalysis, is considered as one of the key steps for chemical and biological evolutions. However, its very existence remains elusive.

Task Description:

An individual molecule of sodium chlorate (NaClO_3) is symmetric, but its crystal form shows distinctive optical activity. If a solution of sodium chlorate is left undisturbed, hundreds of crystals slowly form as the solvent evaporates. If these crystal are examined under crossed polarizers, one finds that half are left-handed and the other half are right-handed. Equal percentages of the two species indicates that the energy barrier for the nucleation is the same for the different handedness. It was discovered by Kondepudi *et al* that under gentle stirring condition the crystallization seems to proceed in one direction, favoring either all crystals being right-handed or left-handed for each individual experiment. The optical purity in each experiment is greater than 99%. However, if an ensemble of experiments is carried out under the same conditions, one again finds an equal distribution of left and right-handed species. This remarkable observation indicates that the system undergoes a transition from a totally symmetric state to a totally asymmetric state simply by the introduction of a hydrodynamic flow.

The current experiments are designed to probe two important aspects of the above observations: (1) We would like to know if the transition from the symmetric state to the asymmetric state is an abrupt transition or a smooth one, as the flow parameters are varied; and, (2) To observe the existence of autocatalysis it will be useful to find correlations between the local order parameter $O = (n_L - n_R) / (n_L + n_R)$, averaging over some spatial scale l , and hydrodynamic flow patterns in the system. Here n_L and n_R are the number densities of left- and right-handed crystals on the scale l . Low Reynolds number hydrodynamic convections, such as Taylor-Couette flow and Rayleigh-Bénard convections, provide fertile testing grounds. In these hydrodynamic systems, the flow consists of many local coherent structures, rolls and eddies, and the convective mixing is most effective within these coherent structures.

Task Significance:

Effect of hydrodynamic convection on phase transitions is a significant problem not only for basic science but also for technology. Microgravity provides a unique environment for which some of the above theoretical ideas can be tested. Here minimization of sedimentation is crucial for both the experimental observations and for the theoretical analysis. This study will enrich our general knowledge about nucleation and growth under hydrodynamic flow and may be exploited to produce chirally pure materials.

Progress During FY 1996:

Over the past year we have carried out extensive measurements aiming at clarifying the physical origin of secondary nucleation in supersaturated sodium chlorate solution under controlled shear flow. Earlier experiments by Kondepudi [1] and by ourselves [2] clearly indicate that explosive growth of these secondary nuclei is responsible for the symmetry breaking. Our new results indicate that mechanical damage to the incipient nuclei is the dominate feature of chiral symmetry breaking, and the secondary nucleation is therefore not spontaneous, contrary to early speculations. We noted that the effect of contact interaction between nuclei and stirrer has been previously investigated [3]; yet the severity of the effect has not been fully recognized. By varying the shear rate continuously and using samples with different amounts of solutions, we showed that the degree of chiral symmetry breaking can be approximately tuned. Moreover, when the flow is generated by means of electric convection, rather than mechanical stirring, no chiral symmetry breaking can be observed [4].

The second issue of concern for this experiment is the mixing effect due to hydrodynamic convection. As noted in our previous report, hydrodynamic convection is a significant problem in a wide range of phenomena concerning transport of pollutants in geostrophic flow, heat transfer in turbulence, as well as phase transitions in fluids. In light of this we have spent a considerable effort in investigating how a passive scalar, any physical quantity (such as the distribution of a dye, temperature or nucleated crystals) that is strongly effected by the flow yet has no or negligible influence on the velocity field itself, is dispersed in a chaotic flow. To simplify the problem, the flow is confined in a plane using very thin liquid (soap) films that are freely suspended. An ingenious technique, similar to that of three-dimensional Couette cells, has been developed to drive the liquid films in a controlled fashion [5]. Both laminar and chaotic flow can be generated using this apparatus. In the chaotic flow regime, it was observed that film thickness variations are coupled strongly to the fluctuating velocity field. A semi-quantitative calculation suggests that film thickness can be treated as a passive scalar. The measured structure function $S(k)$, which is the Fourier transformation of two-point thick-thickness correlation function, is in remarkable agreement with Batchelor's calculation for small scale structures of a passive scalar subject to turbulence flow. The result of this work has been recently published in Phys. Rev. Lett. [5]. A more extensive work which includes statistical properties of velocity fluctuations in the 2D Couette flow is currently underway.

The apparatus that we built not only allows us to study flow in two dimensions, but also allows to characterize physical properties of liquid films. Among various flow parameters, the shear viscosity is perhaps one of the most important ones. Yet, to our knowledge this quantity has never been carefully characterized in freely suspended films. The shear viscosity measurements gave rise to a number of surprises that were not accounted for by current theory. The film viscosity work has just appeared in Rev. Sci. Instr. [6]. We are confident that our study in thin film flow is a new, promising research initiative and will stimulate further theoretical and experimental investigations in this area.

- [1] D.K. Kondepudi, R. Kaufman, and N. Singh, Science, vol. 250, p 975 (1990).
- [2] X-l. Wu, B. Martin, and A. Tharrington, Second Microgravity Fluid Physics Conference Proceedings, NASA Conference Publication 3276, p 319.
- [3] D.K. Kondepudi and C. Sabanayagam, Chem. Phys. Lett., vol. 217, p 364 (1994).
- [4] B. Martin, A. Tharrington, and X-l. Wu, Chiral Symmetry Breaking in Crystal Growth: Is Hydrodynamic Convection Relevant? Phys. Rev. Lett., vol. 77, p 2826 (1996).
- [5] X-l. Wu, B. Martin, H. Kellay, and W.I. Goldburg, Hydrodynamic Convection in a Two-dimensional Couette Cell, Phys. Rev. Lett., vol. 75, p 236 (1995).
- [6] B. Martin and X-l. Wu, Shear Flow in a Two-dimensional Couette Cell - A Technique for Measuring the Viscosity of Free-standing Liquid Films, Rev. Sci. Instr., vol. 66, p 5603 (1995).

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION:	6/93	EXPIRATION:	7/96
PROJECT IDENTIFICATION: 962-24-08-12			
NASA CONTRACT No.: NAG8-959			
RESPONSIBLE CENTER: MSFC			

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Martin, B., and Wu, X-l. Shear Flow in a Two-dimensional Couette Cell - A Technique for Measuring the Viscosity of Free-standing Liquid Films. Rev. Sci. Instr., vol. 66, 5603 (1995).

Martin, B., Tharrington, A., and Wu, X-l. Chiral Symmetry Breaking in Crystal Growth: Is Hydrodynamic Convection Relevant? Phys. Rev. Lett., vol. 77, 2826 (1996).

Wu, X-l., Martin, B., Kellay, H., and Goldburg, W.I. Hydrodynamic Convection in a Two-dimensional Couette Cell. Phys. Rev. Lett., vol. 75, 236 (1995).

Proceedings

Wu, X.-I., Martin, B., and Tharrington, A. Second Microgravity Fluid Physics Conference Proceedings, NASA Conference Publication 3276, p 319.

Presentations

Martin, B. "Thermal convections in a Freely Suspended Soap Films." American Physical Society, March Meeting, San Jose, California, March 1995.

Martin, B. "Two-dimensional Hydrodynamics of Thin Films in Microgravity." NASA Graduate Student Research Program, Washington, DC, May 1995.

Martin, B. "Two-dimensional Thermal Convections in Liquid Films." American Physical Society, Fluid Dynamics Division Annual Meeting, Irvine, California, November 1995.

Oscillatory Thermocapillary Convection

PRINCIPAL INVESTIGATOR: Prof. Abdelfattah Zebib

Rutgers University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The main objective of this work is to investigate the influence of free-surface deflection on the onset of oscillatory thermocapillary convection in microgravity. The study is to investigate the flow instability of thermocapillary flow. The Hopf bifurcation will be studied using a numerical method with the consideration of free-surface deflection. In addition, the disappearance of the Hopf bifurcation will be investigated.

Task Description:

In the domain perturbation approach (valid for small capillary numbers ($Ca \rightarrow 0$)), time-dependent, two-dimensional combined buoyant thermocapillary motions in a rectangular cavity are computed using a second-order accurate finite-volume method. Two situations are investigated: The $O(1)$ pure buoyant convection (with the Marangoni number $Ma=0$) is known to exhibit a Hopf bifurcation at some critical value of the Grashof number, Gr_{cr} . Thus, by studying the combined thermocapillary-buoyant convection for values of

$$(Ma, Gr) \text{ near } (0, Gr_{cr})$$

we seek to determine the stability boundary for onset of oscillatory motion and its nature in the limit of vanishing buoyancy, $Gr=0$. Both positive and negative values of Ma are considered. In the second problem we consider pure thermocapillary driven convection ($Gr=0$). The solution to the zeroth order system is known to be stationary. Higher order effects are unknown and will be investigated.

Task Significance:

These studies can contribute to our fundamental understanding and potential control of thermocapillary instabilities. Detailed information of thermocapillary flows can be obtained through this comprehensive numerical study. Mechanisms for controlling the flows will be identified. Thus the fluid management and heat transfer processes will be better controlled in space.

Progress During FY 1996:

We have computed 2D stability boundaries in the Marangoni number (Ma) - Aspect ratio (A) plane for transition to oscillatory convection in a rectangular cavity assuming a nondeformable interface. We have also considered the influence of the Prandtl number Pr , in the range $1 \leq Pr \leq 10$, and find that the boundaries move in the direction of increasing A and Ma as Pr is decreased. We have also done studies based on the energy method to help understand these transitions. At this time we are generating stability boundaries for $Pr < 1$ as well as carrying out 3D simulations to assess their influence on our 2D stability boundaries. An ASME-IMECE paper has been accepted and will be presented in November 1996. A journal article is under preparation. Mr. Jieyong Xu is the graduate student doing the work as part of his doctoral research.

In previous years, Mundrane & Zebib had demonstrated that thermocapillary convection of small Pr fluids is steady for a range of Ma . They had also shown that surface deflection has a small effect on the motion as expected for small Capillary numbers. In an attempt to explain the apparent discrepancy between space experiments and both theory and ground experiments I have performed a study which has shown that the Coriolis force resulting from the orbiting motion of a space laboratory must be taken into consideration when designing experiments to test oscillatory thermocapillary transitions.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 2/93 EXPIRATION: 2/96

PROJECT IDENTIFICATION: 962-24-05-49

NASA CONTRACT NO.: NAG3-145

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Mundrane, M. and Zebib, A., Low Prandtl number Marangoni convection with a deforming interface. AIAA Journal of Thermophysics & Heat Transfer, 9, p 795-797 (November 1995).

Presentations

Jieyong, X. and Zebib, A., "Oscillatory thermocapillary convection." Third Microgravity Fluid Physics Conference, Cleveland, OH, June, 1996.

Xu, J. and Zebib, A., "Stability analysis of thermocapillary convection in rectangular cavity ." ASME-IMECE, Atlanta, GA, November, 1996.

Xu, J. and Zebib, A., "Nonlinear stability of thermocapillary convection in a rectangular cavity." 48th Annual Meeting of the APS/DFD, Irvine, CA, November 19-21, 1995.

Zebib, A., "Thermocapillary instabilities with system rotation." 49th Annual Meeting of the APS/DFD, Syracuse, NY, November 24-26, 1996.

Superfluid Transition of ^4He in the Presence of a Heat Current

PRINCIPAL INVESTIGATOR: Prof. Guenter Ahlers

University of California, Santa Barbara

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this project is to study the superfluid transition in a heat current. One issue which we are addressing is whether the superfluid transition remains continuous in the presence of a heat current. A second objective is to make measurements of the effective conductivity of the system very close to but slightly above the transition temperature T_λ as a function of the current.

Task Description:

Theoretical work by Onuki has predicted that the transition will be hysteretic. We are looking for this hysteresis in a finite current. Onuki's theory does not take the effect of gravity into consideration, and it is not clear to what extent the gravitationally induced inhomogeneity will hide the predicted effect. Recent calculations by Haussmann and Dohm have indicated that a nonlinear range of parameter space should be accessible where the conductivity will depend upon the current. This range will be exceedingly close to T_λ where the ultra-high resolution thermometry developed previously in our laboratory will be essential, and where gravity effects will play an important role.

Task Significance:

We expect that our earth-bound measurements will yield information about possible advantages to be gained from microgravity experiments. We will have to determine whether gravity effects completely obscure the nonlinear regime, thus necessitating microgravity experiments in order to make these nonlinear effects observable, or whether useful information can be obtained in an earth-bound laboratory.

Progress During FY 1996:

During the time period from our last progress report in November 1995 and the termination of this grant on Dec. 31, 1995 we have continued to study the finite heat current effect on the thermal conductivity of ^4He near the λ transition. Here we briefly describe the problem, and then outline the progress which has been made during the duration of this grant.

The superfluid transition of ^4He has long been a testing ground for theories of critical phenomena. Particularly interesting have been the transport properties. When the transition temperature T_λ is approached from above, the finite conductivity l of the fluid diverges. The precise behavior of l as a function of $t = 1 - T/T_\lambda$ has been studied in great detail both by experiment and theoretically. As T is decreased below T_λ , the effective conductivity remains infinite because the heat current Q is carried by superfluid counterflow. The focus of recent work has been on the behavior as Q is increased beyond the point where linear response theory applies. The properties of phase transitions under such non-equilibrium conditions are relatively unexplored, even though they are an important problem in condensed-matter physics. It is well known that thermal gradients in the superfluid phase can be established by a sufficiently large Q due to the generation of vortices. At even larger Q , it is expected that the superfluid counterflow should become (thermodynamically) unstable even if vortices were absent. A number of early attempts have been made to describe this instability theoretically, but experimental evidence for it remains scarce. Recently, a quantitative prediction, based on the renormalization-group theory, of the line $T_\lambda(Q)$ of absolute instability of the superflow in the T - Q plane has been made by Haussmann and Dohm. This line has much in common with the spinodal line of equilibrium first-order phase transitions. When approaching it from below, one should not expect to reach it because fluctuations will induce a transition at a lower temperature, say at $T_c(Q) < T_\lambda(Q)$. However, there is no theoretical prediction of $T_c(Q)$ and about the nature of the state which will be reached beyond it.

With support from NASA, we discovered an intermediate dissipative region and obtained experimental measurements of its width and thermal resistance in the range $T_c(Q) < T < T_\lambda$. The thermal resistance is much

larger than expected from dissipation due to vortices, but still much smaller than typical thermal resistances in the normal phase above $T_\lambda(0)$. Let us consider a typical example for $Q @ 40 \text{ mW/cm}^2$. Proceeding from high T , the resistivity plummets towards zero near $T_l(Q)$ which is about two mK below $T_\lambda(0)$. The new dissipative region corresponds to the range $T_c(Q) < T < T_\lambda(Q)$ with $T_\lambda(Q) - T_c @ 5 \text{ mK}$. In the new dissipative region the resistivity is over an order of magnitude smaller than it is a mK or so above $T_\lambda(Q)$. However, the resistivity expected from mutual friction (vortices) is several orders of magnitude smaller than the measured resistance.

Since the beginning of this grant, we made measurements in five different cells with different spacings between parallel top and bottom plates. A consistent picture has emerged from them and previous measurements by others. It is as follows. -- As the superfluid transition is approached from below in the presence of a heat current, vortices are generated above a critical temperature relatively far below T_λ . Although in principle thermal gradients are associated with them, these gradients are relatively small. At a temperature somewhat below $T_\lambda(Q)$, the superfluid counterflow which carries the heat current Q becomes thermodynamically unstable and a new phase is entered. The nature of this phase is not very well known, but we find that it has a thermal conductivity much smaller than that of the superfluid state with vortices but an order of magnitude larger than that of the normal fluid. This dissipative state persists until the temperature $T_\lambda(Q)$ of absolutely unstable superflow is reached. At that point the thermal conductivity rises dramatically to values characteristic of the normal fluid.

Our measurements have a direct relationship to the NASA-sponsored microgravity experiment Critical Dynamics in Microgravity Experiment (DYNAMX), which hopes to explore the behavior of the superfluid transition in the presence of a heat current at very small currents where gravity plays an important role. We hope that our results will be helpful in choosing the detailed parameter ranges of DYNAMX.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 1/93 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-24-07-17

NASA CONTRACT NO.: NAGW-33

RESPONSIBLE CENTER: JPL

The Superfluid Transition of ^4He under Unusual Conditions

PRINCIPAL INVESTIGATOR: Prof. Guenter Ahlers

University of California, Santa Barbara

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

One objective of this project is to study the superfluid transition in a heat current. We wish to determine the nature of the transition and the properties of the system near it, and to compare these results with recent renormalization-group calculations. A second objective is to determine the effect of confinement of the sample in finite geometries on the transition. A comparison with ongoing theoretical calculations will shed light on the boundary conditions which pertain to the fluid-solid interface.

Task Description:

We propose to continue our work, previously supported by NASA Grant NAGW-3325, on the superfluid transition in a heat current. During the last funding cycle, we made two major advances of our fundamental understanding of this topic. First, we found that there is no hysteresis of the transition in a heat current, contrary to early theoretical predictions. Second, we discovered a new dissipative phase below the usual transition temperature $T_\lambda(Q)$ with properties quite different from those typical of the expected Gorter-Mellink-Vinen mutual friction between the normal fluid and the superfluid. We now propose to study the properties of this phase in greater detail, and to extend the heat-current range of our measurements. This work has a direct bearing on the proposed flight experiment DYNAMX, which will probe similar phenomena in smaller heat currents where the effects of interest occur so close to the zero-current T_λ as to be obscured in the earth's gravity. We expect our work to yield new fundamental scientific results and to be relevant to the detailed choice of parameter values for the DYNAMX experiment.

As a second line of investigations we propose to measure thermodynamic and transport properties in confined geometries. This work will be complementary to presently planned and future finite-size micro-gravity experiments, such as the Confined Helium Experiment CHEX, which is well advanced at this time. In particular, we expect to measure the thermal conductivity and the heat capacity of helium near the superfluid transition in cylindrical geometries with diameters ranging from 2 to 50 mm. Our present understanding of finite-size effects is rapidly advancing, largely through the efforts of Professor Dohm who is closely associated with the fundamental-science effort within MSAD. We expect our measurements to provide quantitative tests of these emerging theoretical predictions. This comparison between theory and experiment will provide crucial tests of current ideas about such fundamental issues as the nature of the boundary conditions which are appropriate for the treatment of the solid-liquid interface near a phase transition. We expect this ground-based effort to be complementary to the microgravity experiment CHEX.

Task Significance:

We expect that our Earth-bound measurements will yield information about possible advantages to be gained from microgravity experiments. We will have to determine whether gravity effects completely obscure the nonlinear regime, thus necessitating microgravity experiments in order to make these nonlinear effects observable, or whether useful information can be obtained in an Earth-bound laboratory. We expect our measurements in a finite heat current to be relevant to the microgravity experiment DYNAMX. Similarly, our finite-size experiments will complement the information to be derived from the microgravity experiment CHEX.

Progress During FY 1996:

Since May, 1996 we have continued to study the finite heat-current effect on ^4He near the superfluid transition at T_λ . We constructed a new multi-purpose experimental cell which is now being used to investigate the boundary (Kapitza) resistance R_b between the liquid helium and a solid surface. This cell has two sideplanes which make it possible to determine the actual helium temperature at two different vertical positions. High-resolution thermometers are located on the side planes, as well as on the cell top and bottom. Previous work in our laboratory had revealed that, even in the zero-current limit, R_b has a singularity near T_λ . We, as well as others, also found that

there is a large finite-current contribution to measurements of R_B . The group at Duke University discovered recently that the finite-current contribution is not intrinsic, but rather is due to the gap between the copper anvil and the sidewall at the cell ends which has existed in previous cells. We confirmed this result. Our cell has such a gap at one end, but not at the other. Because of the side-plane thermometers, we are able to measure R_B separately at each end. At the end with the gap, the finite-current effect exists. At the other, only the zero-current singularity was found. We are now in a position to make measurements of the zero-current singularity which are much more precise than previous ones because we can now use much larger currents. Our new results are more precise than, but are consistent with, the previous measurements in our laboratory by Duncan, et al.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/96 **EXPIRATION:** 5/00

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NAG3-184

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Liu, F.-C., and Ahlers, G. A new dissipative region below the superfluid transition of 4He in a heat current. *Physical Review Letters*, vol. 76, 1300 (1996).

Proceedings

Ahlers, G. and Liu, F.-C. "4He very near Tl heated from above." *Proceedings of the 21st International Conference on Low Temperature Physics LT-21 (Prague)*, Czechoslovak Journal of Physics, vol. 46-Suppl, 187 (1996).

Baddar, H., Fu, H., Larson, M., Mulders, N., and Ahlers, G. "A High-Resolution Susceptibility Thermometer for use Near 2 K." *Proceedings of the 21st International Conference on Low Temperature Physics LT-21 (Prague)*, Czechoslovak Journal of Physics, vol. 46-Suppl, 2859 (1996).

Baddar, H., Fu, H., Liu, F.-C., and Ahlers, G. "The Thermal Boundary Resistance in Superfluid 4He Near Tl." *Proceedings of the 21st International Conference on Low Temperature Physics LT-21 (Prague)*, Czechoslovak Journal of Physics, vol. 46-Suppl, 191 (1996).

Baddar, H., Fu, H., Liu, F.-C., and Ahlers, G. "The Thermal Boundary Resistance of 4He near Tl." *Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop*, NASA Document D-13845.

Fu, H., Baddar, H., Larson, M., Mulders, N., and Ahlers, G. "A high-resolution thermometer using a DC SQUID." *Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop*, NASA Document D-13845.

Liu, F.-C., and Ahlers, G. "Thermal Resistance below the Superfluid Transition of 4He in a Heat Current." *Proceedings of the 21st International Conference on Low Temperature Physics LT-21*, Czechoslovak Journal of Physics, vol. 46-Suppl, 189 (1996).

Liu, F.-C., and Ahlers, G. "4He very near Tl heated from above." *Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop*, NASA Document D-13845.

Microgravity Test of Universality and Scaling Predictions Near the Liquid-Gas Critical Point of ^3He

PRINCIPAL INVESTIGATOR: Dr. Martin B. Barmatz

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Hahn, I.

Jet Propulsion Laboratory (JPL)

Israelsson, U.E.

Jet Propulsion Laboratory (JPL)

Rudnick, J.

University of California, Los Angeles

Task Objective:

The objectives of this task are to test the universality and scaling laws at the liquid-gas critical point of ^3He in a microgravity environment. The task objectives will include 1) precision measurements of the isothermal compressibility along the critical isochore to determine the critical exponent and 2) precision measurements of the constant volume specific heat along the critical isochore to determine the critical exponent α , and 3) sound attenuation and dispersion measurements to test dynamic scaling theories.

Task Description:

Theories describing the behavior of thermophysical properties near critical points were developed using the concept of scaling laws. These models led to the definition of universality classes where critical points of the same class are predicted to have the same critical exponents. Efforts to validate the scaling law predictions near a liquid-gas critical point in ground-based laboratories are limited due to the gravity-induced vertical density gradient associated with the divergence of the isothermal compressibility. This density gradient becomes appreciable as the critical point is approached, leading to a significant smearing of the transition. Calculations have shown that in a microgravity environment (10^{-6} g) accurate specific heat and isothermal compressibility measurements could be obtained two orders of magnitude in reduced temperature closer to the critical point. Techniques are being developed for the simultaneous measurement of both static (specific heat, sound velocity, and compressibility) and dynamic (sound attenuation and dispersion) properties. These studies will require accurate measurements of pressure ($\Delta p/p \sim 10^{-11}$), density ($\Delta \rho/\rho \sim 10^{-9}$), and temperature ($\Delta T/T \sim 10^{-9}$). These simultaneous measurements in microgravity should provide a very stringent test of theoretical predictions.

Task Significance:

The ability to perform these simultaneous measurements in microgravity should provide a very stringent test of the universality predictions.

Progress During FY 1996:

During this last year, we designed and fabricated a heat capacity cell for the ^3He critical point experiment. This cell has three capacitive density sensors for measuring the density of the fluid and for leveling the cell in a gravitational field. We are currently mounting the cell on the high resolution thermometer stage of the thermal control system. For thermal control, we have implemented a new fuzzy gain scheme in a proportional-integral-differential (PID) controller. Computer simulations show that the new controller settles faster with less overshoot than a regular PID controller. Testing is now in progress with the real system containing high resolution thermometers. We have also collaborated with Dr. Ulf Israelsson to evaluate a high resolution pressure gauge for compressibility measurements near the critical point that is based on silicon micromachining technology.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 12/92 EXPIRATION: 11/95

PROJECT IDENTIFICATION: 962-24-04-07

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Cowan, M., Rudnick, J., and Barmatz, M. Effects of random motions on critical point measurements: liquid-gas systems in microgravity. *Physical Review E*, vol. 53, 4490 (1996).

Proceedings

Hahn, I., Gonzalez, A., and Barmatz, M. "Fuzzy logic controller for low temperature applications." Proceedings of the 21st International Low Temperature Physics Conference LT-21 (Prague), Czechoslovak Journal of Physics vol. 46 (1996).

New Phenomena in Strongly Counterflowing He-II near T_λ

PRINCIPAL INVESTIGATOR: Dr. Stephen T. Boyd

University of New Mexico

CO-INVESTIGATORS:

Duncan, R.V.

Strayer, D.

Adrianns, M.J.

University of New Mexico

Jet Propulsion Laboratory (JPL)

Sandia National Laboratories

Task Objective:

We intend to study strongly flowing superfluid helium near the transition temperature T_λ . Our objectives are to study two important problems: First, to investigate the new regime of thermal resistance in helium just below the transition recently discovered by Liu and Ahlers; and second, to investigate recent predictions of nonlinear phenomena, such as thermal solitons, when counterflow is strong enough to render the superfluid helium thermodynamically unstable.

Task Description:

To perform these measurements, we shall construct a thermal conductivity cell that incorporates four recently proven techniques: 1) SQUID-based paramagnetic salt thermometry; 2) wet thermometry; 3) sidewall thermometry; and 4) a numerically optimized geometry of the SQUID pick-up coils and the magnetic shields to eliminate cross-talk between two wet thermometers. Additionally, the cell will be constructed with a varying cross-section, necking to smaller diameter at the middle, to permit access to higher counterflow velocities in single-phase samples of helium.

Task Significance:

Our measurements will further elucidate the complex thermodynamics of liquid helium near T_λ , and will contribute to the fund of high-quality data on critical behavior in highly nonequilibrium systems.

Progress During FY 1996:

Funding is presently being put in place. Work will begin in very late FY96 or early FY97. The work which could occur in very late FY96 would be initial design definition.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/96 EXPIRATION: 10/00

PROJECT IDENTIFICATION:

RESPONSIBLE CENTER: JPL

Prediction of Macroscopic Properties of Liquid Helium from Computer Simulation

PRINCIPAL INVESTIGATOR: Prof. David M. Ceperley

University of Illinois, Urbana-Champaign

CO-INVESTIGATORS:

Goldenfeld, N.

University of Illinois, Urbana-Champaign

Task Objective:

The aim of this research is to provide reliable, quantitative theoretical predictions which will aid in the design and interpretation of low temperature experiments performed in the microgravity facility. Considerable progress can be achieved on these fronts, owing to the possibility of performing accurate measurements in a gravity-controlled environment and making comparison with state-of-the-art numerical calculations.

Task Description:

In the first year we plan accurate simulations, based on realistic interatomic potentials, of bulk superfluid, droplets, and helium mixtures at finite temperature, as well as macroscopic simulations of the large-scale dynamics of liquid helium using microscopically calculated parameters as input.

We plan to extend the capabilities of our Path Integral Monte Carlo code to do simulations of systems relevant to NASA's experimental low temperature program: to extend the numerical investigation to systems several orders of magnitude larger than we can presently handle; more precisely, our goal is to simulate systems composed of as many as several thousand helium atoms, an order of magnitude more than at present. This will enable us to study how the macroscopic description emerges from the microscopic interactions, by investigating long-range spatial and momentum correlations and vortex-vortex interactions, as well as droplets of an experimentally relevant size.

We will also adopt cell dynamical system (CDS) techniques, to perform calculations of vortex dynamics in superfluid helium in the regime of nonlinear drag force. We will seek to understand the onset of turbulent drag and the sources of dissipation in the weakly turbulent regime.

Task Significance:

This research is concerned with fundamental aspects of helium and quantum fluids in general; we plan to address outstanding problems in the current understanding of relevant phenomena such as Bose condensation, superfluidity, and phase transitions, as well as of theoretical issues such as the inference of bulk properties of matter from the study of finite clusters. The theoretical issues involved in helium systems are of direct relevance to understanding other many-body quantum systems such as correlated electronic systems.

Progress During FY 1996:

This task is new, so no progress has been made to date.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/96 **EXPIRATION:** 7/00**PROJECT IDENTIFICATION:****NASA CONTRACT NO.:** NAG3-192**RESPONSIBLE CENTER:** JPL

Measurement of the Heat Capacity of Superfluid Helium in a Persistent-Current State

PRINCIPAL INVESTIGATOR: Dr. Talso C. Chui

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of the task is to detect any changes in the heat capacity of helium as result of superfluid flow very near the superfluid transition temperature.

Task Description:

The flow in the form of persistent current will be created in a toroidal-shaped calorimeter. The heat capacity is then measured from below to above the transition, where the persistent current will decay to zero. The heat capacity will subsequently be remeasured below the transition to detect any difference. If the experiment shows that the heat capacity is different with superfluid flow, then a space experiment can be designed to map out the heat capacity curves as a function of temperature and superfluid velocity.

Task Significance:

The results will be compared to the renormalization group (RG) theory, which has recently been applied to calculate the expected behavior. Although RG theory has been remarkably successful in explaining many properties of matter near a phase transition, the effect being studied here is a unique manifestation of quantum properties of superfluid helium. The theory developed to explain this involves a way to combine RG theory and quantum mechanics through the use of the Josephson relation. The experiment will examine whether such an extension of RG theory will correctly describe nature.

Progress During FY 1996:

In an attempt to understand the theory behind the experiment, we have discovered a major discrepancy with the theoretical predictions. We found that under superfluid flow the heat capacity is different, depending on what parameter is held constant during the measurement. This is analogous to the heat capacity at constant volume versus the heat capacity at constant pressure. In superfluid flow, one can either hold the superfluid velocity constant or the applied heat current constant. Previously, it was thought that both cases would give the same heat capacity. We found that the case of constant heat current would give a much larger heat capacity, and therefore its effect is much more easily detected. Our calculation was published in Physical Review Letters.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 12/92 EXPIRATION: 11/95

PROJECT IDENTIFICATION: 962-24-04-08

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Goodstein, David, Chui, Talso C. P., and Harter, Alexa Heat flow induced anomalies in superfluid 4He near T_l. Physical Review Letters, 77, 979 (1996).

Proceedings

Chui, Talso C. P., Goodstein, David L., Harter, Alexa W., and Mukhopadhyay, Ranjan "Heat Capacity of Superfluid 4He in the Presence of a Heat Current near T_l." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13485 (1996).

Nonequilibrium Phenomena Near the Lambda Transition of ^4He

PRINCIPAL INVESTIGATOR: Dr. Talso C. Chui

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Israelsson, U.E.

Jet Propulsion Laboratory (JPL)

Task Objective:

The objective of this project is to obtain information on the order-parameter relaxation time in superfluid helium near the lambda transition.

Task Description:

We attempt to measure the temperature change in helium following a sudden application of pressure. The pressure quench is applied by a piezoelectric piston. The decay of the temperature to a lower equilibrium value after the sudden pressure increase will give a direct measurement of the order parameter relaxation time. This approach requires the use of a very fast bolometer. Since the relaxation time is predicted to slow down considerably near the transition, getting closer to the transition will avoid problems on Earth associated with extremely fast relaxation.

Task Significance:

The order-parameter relaxation time is an important parameter characterizing all dynamic processes in a phase transition. Accurate measurement of this quantity will allow a stringent test of the dynamic renormalization group theory which can be applied to predict the behavior of this quantity with no adjustable parameters.

Progress During FY 1996:

We have completed the fabrication of a cryoprobe for the experiment. A new postdoctoral associate will join our group. The bolometer has been fabricated. Some calculations were performed to understand thermodynamics of helium under a sudden pressure quench.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/94 EXPIRATION: 8/96

PROJECT IDENTIFICATION: 962-24-04-12

RESPONSIBLE CENTER: JPL

The Lambda Transition Under Superfluid Flow Conditions

PRINCIPAL INVESTIGATOR: Dr. Talso C. Chui

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Strayer, D.
Vinen, W.F.Jet Propulsion Laboratory (JPL)
University of Birmingham

Task Objective:

The objective of the task is to detect any changes in the heat capacity of helium as the result of superfluid flow very near the superfluid transition temperature.

Task Description:

There are three scenarios where superfluid flow conditions exist:

- 1) The case of a persistent current around a loop, where the superfluid velocity is kept constant.
- 2) The case of a constant applied heat current, where the superfluid momentum is kept constant.
- 3) The case of superfluid flow around the core of vortices.

Recent theoretical developments by us have shown that the case of constant heat current gives the largest heat capacity changes. Therefore our initial task will concentrate on the measurement of heat capacity under a constant applied heat current.

Task Significance:

Counterflow in a superfluid represents a new degree of thermodynamic freedom only available in a macroscopic quantum system. The effect on the superfluid transition of an imposed counterflow is of contemporary interest.

Progress During FY 1996:

This is a new task funded late in FY96.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/96 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 962-24-04-15

RESPONSIBLE CENTER: JPL

Nucleation of Quantized Vortices from Rotating Superfluid Drops

PRINCIPAL INVESTIGATOR: Prof. Russell J. Donnelly

University of Oregon

CO-INVESTIGATORS:

Niemela, J.
Rhim, W.-K.University of Oregon
Jet Propulsion Laboratory (JPL)

Task Objective:

The objective of this research is to study the nucleation of quantized vortices in helium II by investigating the behavior of rotating droplets of helium II in a reduced gravity environment.

Task Description:

Two methods well-suited for levitating the helium drop in the near vacuum environment are electrostatic and/or magnetic levitation. A pure electrostatic scheme requires active feedback control, while a purely magnetic levitation requires large fields. A hybrid system is probably the best choice. Rotation can be accomplished by coupling to a charge distribution on the drop surface. We will initially use purely electrostatic levitation for studying drops. The required charging of the drops can be accomplished by forming the drops around a sharp electrode tip held at a high voltage. Film flow of helium II can be utilized to create drops at the bottom of a suitable container which can be filled by a fountain pump and situated above a pair of capacitor plates having an appropriate voltage difference between them.

Task Significance:

Nucleation phenomena, in general, are fundamental to many fields of physics and engineering. In the case of a rotating superfluid drop, it will be possible to produce a state of zero nucleation, analogous to growing a perfect defect-free crystal. It should also be possible to add a controlled impurity to cause nucleation of a quantized vortex line in the drop. At low enough temperatures, this nucleation will be a pure quantum mechanical tunnelling phenomenon. At higher temperatures it should be possible to see thermally activated nucleation taking over, for a demonstration of nucleation under more familiar classical conditions. In conventional systems it is evident that vortex lines come from some preexisting source, probably vortices trapped by pinning sites on the walls. While this kind of source of vorticity is undoubtedly important, it is not as fundamental as the "extrinsic nucleation" problem where vortex line appears when none was present before.

Progress During FY 1996:

This year the electrostatic levitation of liquid helium drops has continued to progress. We achieved long-lived levitation of small, positively-charged superfluid droplets using an electrodynamic levitator. By exploring many options for design and operation, the containment time was extended with each run, culminating with drops being suspended for over twenty minutes. Finally, we are currently writing up results of our initial drop levitation studies for submission to the Journal of Low Temperature Physics this year.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	2	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 1/93 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-24-07-12

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Donnelly, R. J. "The Field of Low Temperature Physics." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13485 (1996).

Presentation

Donnelly, R. J. "Low Temperature Physics." The London Lectures, Duke University, March 1996.

Nucleation of Quantized Vortices from Rotating Superfluid Drops

PRINCIPAL INVESTIGATOR: Prof. Russell J. Donnelly

University of Oregon

CO-INVESTIGATORS:

Niemela, J.J.

University of Oregon

Vinen, W.F.

University of Birmingham

Task Objective:

The objective of this research is to study the nucleation of quantized vortices in helium II by investigating the behavior of rotating droplets of helium II in a reduced gravity environment.

Task Description:

We will initially make careful measurements of the dielectric constant, or index of refraction, of the helium. To accomplish this the helium will be confined within a parallel plate capacitor. Measurement of the capacitance will be by means of an audio-frequency bridge circuit. We will employ high resolution paramagnetic salt thermometers to precisely measure the temperature of the sample. By approaching the lambda point temperature closely, and by reducing the size of the capacitor gap, we will be able to make measurements as the coherence length approaches the size of the sample. These gaps will be of order 1-10 microns, which is in the range of droplet sizes we have observed generated in a fine mist.

Task Significance:

Nucleation phenomena, in general, are fundamental to many fields of physics and engineering. In the case of a rotating superfluid drop, it will be possible to produce a state of zero nucleation, analogous to growing a perfect defect-free crystal. It should also be possible to add a controlled impurity to cause nucleation of a quantized vortex line in the drop. At low enough temperatures, this nucleation will be a pure quantum mechanical tunnelling phenomenon. At higher temperatures it should be possible to see thermally activated nucleation taking over, for a demonstration of nucleation under more familiar classical conditions. In conventional systems it is evident that vortex lines come from some preexisting source, probably vortices trapped by pinning sites on the walls. While this kind of source of vorticity is undoubtedly important, it is not as fundamental as the "extrinsic nucleation" problem where vortex line appears when none was present before.

Progress During FY 1996:

We are presently working on development of a thin-film sample capacitor for making accurate dielectric constant measurements. This work is in collaboration with Joel Nissen from John Lipa's group at Stanford University. The electrode surfaces will be niobium deposited on an optically-flat silicon substrate, although initial testing is being done on a glass substrate. Additionally, a high-resolution paramagnetic salt thermometer has been obtained which can be used in our present apparatus with some slight modifications. We have installed and successfully tested a B.T.I. RF SQUID probe for use with this thermometer. We are studying whether a second SQUID could be used advantageously as a cryogenic null-meter in a capacitance bridge. With consultation from Dr. Randall Kirschman, we have designed a cryogenic preamplifier for low frequency (~1kHz) signals. We expect as much as a five-fold increase in bridge off-balance sensitivity resulting from this device. A mechanically-actuated low-temperature valve has been designed for our apparatus and we will be making appropriate modifications to the cryostat to install it.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: NAG3-1934

NASA CONTRACT NO.: NAG3-193

RESPONSIBLE CENTER: JPL

Kinetic and Thermodynamic Studies of Melting-Freezing of Helium in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Charles Elbaum

Brown University

CO-INVESTIGATORS:

Kosterlitz, J.M.

Brown University

Task Objective:

The objective of this project is to study, experimentally and theoretically, the effects of gravity on the melting-freezing transitions, including kinetic processes and the equilibrium shape of solids. The research is carried out on helium, whose unique properties render such investigations possible on a time scale consistent with experiments in space, under microgravity conditions. Indeed, morphological changes of the solid-liquid interface (i.e., the "surface" of helium) generally occur fast enough to satisfy the time constraints mentioned above.

Task Description:

An optical system with special lighting applied to a growth cell contained in a liquid helium dewar allows viewing of the solid-liquid interface (SLI) and of crystal shapes. Rapid image capture equipment allows recording of the evolution of the SLI and of the crystal shapes in response to changes in temperature and pressure.

Task Significance:

These studies are addressing a number of fundamental questions, especially as they relate to the effects of gravity. These questions include the kinetics of first order phase transitions, the critical behavior in the evolution of crystal shapes as they approach equilibrium, faceting-roughening phenomena on various surfaces, relative and absolute values of interfacial free energy for different crystal faces, and the minimization of a system's free energy subject to various constraints. Furthermore, many applications should benefit from a deeper understanding of the above phenomena, among them crystal growth, surface configurations, sintering, and surface reactivity.

In the course of this research we discovered a new phenomenon of nucleation in a first order phase transition, whereby a nonequilibrium phase nucleates and persists in a metastable state. This nucleation occurs from overpressurized superfluid helium-4 into the body-centered cubic (BCC) solid phase, in preference to the expected equilibrium hexagonal close-packed (HCP) phase. These observations provide a new perspective on the kinetics of first order phase transitions occurring near the triple points, and in systems having two or more phases with modest free energy differences.

We are directing a part of our research effort to this newly discovered phenomenon.

Progress During FY 1996:

In the Progress Report for FY95 we described the general background of nucleation and growth processes, and their relation to the solidification of helium. We also discussed, in the same context, our discovery of the nucleation and growth of a non-equilibrium (metastable) phase from overpressured superfluid helium, in preference to the stable phase.

This work on nucleation and growth has continued in FY96. We extended the range of our experiments along the lines described previously. In order to enhance the resolution of our temperature and pressure measurements, we reworked our thermometry set-up and the pressure detection system. We also installed a faster system for the acquisition and processing of video images of the nucleation growth events under study. This system consists of a fast computer with sufficient random access memory (RAM) for storing the real-time information acquired, a high-speed bus interface required for the frame grabber, plus a frame grabber that allows us to digitize video data in real time and to store the information in system memory. This approach allows us to acquire batches of 150 digitized, standard (30 frames/second) video frames in real time.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 0

PhD Students: 1

TASK INITIATION: 1/93 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-24-07-13

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Johnson, T.A. and Elbaum, C. "Nucleation of a non-equilibrium phase in a first-order phase transition: Bcc 4He from superfluid." American Physical Society March Meeting, St. Louis, MO, March 18-22, 1996.

Kinetic and Thermodynamic Studies of Melting-Freezing of Helium in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Charles Elbaum

Brown University

CO-INVESTIGATORS:

Kosterlitz, J. M.

Brown University

Task Objective:

In addition to continuing with the overall objectives for the previous year, in FY 96 we will extend our focus on studies of first-order phase transitions. Particular attention will be directed to nucleation of a non-equilibrium solid phase from liquid helium, that we discovered previously. Our model for explaining this phenomenon is based on effects of the combination of solid-liquid interfacial free energies and bulk free energy differences for the equilibrium and non-equilibrium solid phases relative to those of the liquid. In order to explore the effects of these free energies we will alter their values by extending the range of temperature and pressure of the experiments and possibly by additions of ^3He .

Task Description:

An optical system with special lighting applied to a growth cell contained in a liquid helium dewar allows viewing of the solid-liquid interface (SLI) and of crystal shapes. Rapid image capture equipment allows recording of the evolution of the SLI and of the crystal shapes in response to changes in temperature and pressure.

Task Significance:

These studies are addressing a number of fundamental questions, especially as they relate to the effects of gravity. These questions include the kinetics of first order phase transitions, the critical behavior in the evolution of crystal shapes as they approach equilibrium, faceting-roughening phenomena on various surfaces, relative and absolute values of interfacial free energy for different crystal faces, and the minimization of a system's free energy subject to various constraints. Furthermore, many applications should benefit from a deeper understanding of the above phenomena, among them crystal growth, surface configurations, sintering, and surface reactivity.

In the course of this research we discovered a new phenomenon of nucleation in a first order phase transition, whereby a nonequilibrium phase nucleates and persists in a metastable state. This nucleation occurs from overpressurized superfluid helium-4 into the body-centered cubic (BCC) solid phase, in preference to the expected equilibrium hexagonal close-packed (HCP) phase. These observations provide a new perspective on the kinetics of first order phase transitions occurring near the triple points, and in systems having two or more phases with modest free energy differences.

Progress During FY 1996:

Work has continued on the experiments and apparatus enhancement in the study of nucleation and growth of helium from overpressurized superfluid ^4He . In the period covered by this report, we completed a manuscript for publication entitled "Nucleation of a Non-Equilibrium Phase in a First-Order Phase Transition," by T. A. Johnson and C. Elbaum.

Theoretical Progress

Work is in progress checking that the proposed full phase model for a solid/superfluid system does reduce to more conventional sharp interface equations in the appropriate limit. The free energy functional with the equations of motion do reduce to correct superfluid hydrodynamics in the fluid phase. To make the model more convincing, we are in the process of attempting to derive the well-known dispersion relation for melting/freezing waves from the full phase model. If we can reproduce behavior by assuming a sharp interface between the solid and fluid and integrating the equations of motion across the interface, we shall be able to put some constraints on the phenomenological parameters of the full phase model. The dispersion relation for melting/freezing waves is known to be $\omega^2 = A (\gamma k^3 + b k)$, where A is given in terms of the densities of the liquid and solid, b is proportional to g , the acceleration of gravity, and γ is the surface stiffness, which is just the surface tension for a rough surface. Since the

coefficients of k_3 and k are known experimentally and are given in terms of the model parameters, we have some constraints on these terms. More importantly, that the melting/freezing wave dispersion relation can be derived from the full phase model is a good test of the applicability of the model.

TASK INITIATION: 7/96 EXPIRATION: 7/(X)

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NAG3-192

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Johnson, T. A., and Elbaum, C. Nucleation of a non-equilibrium phase in a first order phase transition. *Journal of Low temperature Physics*, in press, (1996).

Critical Dynamics of Ambient Temperature and Low Temperature Phase Transitions

PRINCIPAL INVESTIGATOR: Prof. Richard A. Ferrell

University of Maryland

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The task objectives are to provide theoretical background and support for the manifested low temperature flight experiments CheX and DYNAMX, as well as for other proposed experiments, such as the study of second sound below the lambda point. The task objectives can be grouped into five categories as follows:

1. Thermal conductivity
2. Critical damping of second sound
3. Specific heat in confining geometry
4. Critical Kapitza resistance
5. Superconductivity analogies

Task Description:

1. Thermal Conductivity

There is strong incentive to move out of the quasicaling region and closer to the lambda point and the true asymptotic region by a flight experiment (DYNAMX, R. Duncan, P.I.). At the 1987 Oregon Low Temperature Workshop, I (and A. Onuki, independently) noted that one can "beat" gravity by heating the liquid helium from above so as to establish a temperature gradient that exactly matches the gradient in T_1 coming from gravity. This gradient cancellation will insure that $DT = T - T_\lambda$ will be the same at every point. The price to pay is that, as $DT \rightarrow 0$, the diverging heat current takes us into a nonlinear region, requiring an extension of the theory beyond linearity. By means of a kinetic theory type reformulation of critical dynamics theory, similar to that employed for parasuperconductivity in a strong electric field, we found that the nonlinear correction to the theory is not very drastic. We propose continuing this theoretical investigation as a kind of ground-based support for the thermal conductivity flight experiment DYNAMX.

2. Critical Damping of Second Sound

As T is lowered below T_λ , any resistance to heat flow (in the linear region) disappears and the relevant dissipative non-equilibrium property to study is the damping (and dispersion) of second sound. At the same time we predicted the divergence above T_λ we also predicted a similar divergence approximately as $(T - T_\lambda)^{-1/3}$ in the coefficient of attenuation of second sound below T_λ . The theory of this effect is much less advanced than the theory of the thermal conductivity for $T > T_\lambda$. We therefore propose to attack the computation of the higher loop ϵ -expansion contributions with the able help of Visiting Professor Jayanta K. Bhattacharjee.

3. Specific Heat in Confining Geometry

Although this is not a topic in critical dynamics, but rather a problem in equilibrium statistical physics, it is a subject of great current interest because of the forthcoming space experiment CheX (J. Lipa, P.I.). In our paper entitled "An Experimental Prediction for CheX" (J. K. Bhattacharjee and R. QA. Ferrell, Procs. NASA Low Temperature Physics Workshop, Washington, D.C., January 1994, eds. Ulf Israelsson and Don Strayer), we used the method of images to relate the light scattering data with what should be expected from the confinement between plates of separation L . We developed the connection with light scattering at odd multiples of transfer number $kL = p/L$ (i.e. for $kn = np/L$, where $n = \text{odd integer}$). During the past few months we have been examining the approximations involved in the image method and we propose to carry this study through to completion, with special attention to the effect of confinement on the order parameter.

4. Critical Kapitza Resistance

This subject is closely related to item #1 above, as the Kapitza resistance generally plays an important role in the interpretation of measurements of the thermal conductivity. We shall be using the theoretical approach that we described in the proceedings of the International Low Temperature Physics Conference (Brighton, 1990).

5. Superconducting Analogies

Techniques developed in the theory of superconductivity will be applied to understanding superfluidity better.

Task Significance:

1. Thermal Conductivity

The divergence in the thermal conductivity as T approaches T_λ , the lambda point temperature, from above was predicted by our group to vary, approximately as $x^{1/2}$, or as $(T - T_\lambda)^{-1/3}$. This result was also the first example of dynamic scaling theory which we and others subsequently extended to other second-order phase transitions, such as those that occur in classical fluids, ferromagnets, antiferromagnets, etc. The lambda point continued to be a strong interest of ours, and we demonstrated that the apparent discrepancy between dynamic scaling theory and the experimental data for the thermal conductivity resulted from a very slow and strong transient, i.e. a correction to scaling. The experiments were carried out in a "quasiscaling" region where the divergence is somewhat stronger than predicted by the asymptotic dynamic scaling theory. Our computation will be relevant for DYNAMX, which will approach the asymptotics more closely.

2. Critical Damping of Second Sound

Second sound damping offers a test of the theory of critical dynamics below the lambda point that has a potential significance that is equivalent to that provided by the thermal conductivity above the lambda point. Unfortunately, the theory is much more complicated below the lambda point, and requires much more work to realize its potential. In addition to this effort, we plan to study to what extent the study of the thermal surface impedance might provide an interesting comparison between theoretical predictions and the data from ground-based experiments. The idea to pursue here is that the active layer of the fluid in contact with the horizontal surface of the transducer of second sound might be kept thin enough to avoid the complications of gravity. In the first qualitative applications of dynamic scaling theory to the lambda transition, the prediction for second sound damping was on a par with the prediction for the divergence of the thermal conductivity. But as the theory was refined, more attention came to be given to the thermal conductivity. The thrust of this part of the project is to invest enough theory effort into the complicated and difficult problem of second sound damping so as to bring it back to parity as a quantitative proving ground for theory with experiment. This is particularly timely now that advanced experimental techniques have been developed that permit coming much closer to the lambda line from below. The calculations will be relevant for the later flight experiment by the group of J. Lipa.

3. Specific Heat in Confining Geometry

The comparison of the predicted shift and rounding of the lambda-point specific heat peak with the data from CHeX will be a rigorous and significant test of the theory of phase transitions.

4. Critical Kapitza Resistance

The observed thermal resistance of a cell of liquid ^4He is the sum of bulk and surface contributions. Because of the critical behavior of the latter, it will be essential to have a reliable theory of it so as to be able to disentangle and separate the true bulk behavior from the DYNAMX data.

5. Superconductivity Analogies

The properties of both the superfluid and normal fluid components in liquid ^4He below the lambda point have their counterparts in superconductivity. Exploring these similarities will give useful insight into superfluidity.

Progress During FY 1996:

In contrast to the binary fluids, the order-parameter relaxation rates in the pure fluids are greatly affected by a large non-critical component. With the appropriate cross-over correction to dynamic scaling, we restore universality and demonstrate that the ultrasonic data for both the one- and two-component fluids fall on the same scaling plot.

A particularly significant and attractive feature of critical phenomena is the universality exhibited by widely different physical systems, provided only that they belong to the same universality class. This, indeed, can be regarded as the hallmark of critical behavior. This universality, encompassing pure fluids as well as binary liquids, is contained in the general theory of critical ultrasonic attenuation that is based on an extension of the concept of frequency-dependent specific heat. In this method, used in its original form by Herzfeld and Rice for the ultrasonic attenuation in gases, the dominant frequency dependence for a fluid near its critical point, as noted by Fixman, comes from the critical slowing down of the fluctuations of the order parameter. A small portion of a recent Physical Review Letter by us reports on a computation of the ultrasonic attenuation in liquid ^3He near its critical point. In this very brief announcement, no attention is paid to universality and no comparison is made with other fluids. The purpose of the discussion here is to emphasize that such a restriction to one particular fluid is not only unnecessary but, furthermore, sacrifices the advantages offered by the broad concept of universality. We will demonstrate explicitly how the very same scaling function which has yielded excellent agreement with the ultrasonic data of Garland and Sanchez for a binary liquid near room temperature also accounts for the ultrasonic data in the low temperature pure fluid liquid ^3He .

Prof. Bhattacharjee has developed a method for taking into account the effect of boundary conditions on order parameter fluctuations, with a view toward making a prediction for CheX.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION:

NASA CONTRACT No.: NAG3-186

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Ferrell, R. A. "A brief survey of the equilibrium and transport properties of critical fluids and the degree to which microgravity is required for their experimental investigation." Proceedings of the Third Microgravity Fluid Physics Conference, Cleveland, June 1996, NASA conference publication 3338, 53-57 (1996).

Presentations

Ferrell, R. A. "Modulated order parameter." Max Planck Institut fuer Physik Komplexer Systeme, Dresden, Germany, June 1996.

Dynamics of Superfluid Helium in Low Gravity

PRINCIPAL INVESTIGATOR: Mr. David J. Frank

Lockheed Martin Missiles & Space Co.

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this project is to simultaneously record the 3-axis acceleration time history and make a video recording of the position of superfluid helium (SFHe) in a test cell while in a low-gravity environment. This data can then be used as a benchmark for validation of a 3-D CFD simulation of SFHe flow behavior.

Task Description:

The first part of the project is to build a SFHe dewar and a support equipment package to allow operation of the dewar and recording of 3-axis accelerations and video images of the fluid motion on the DC-9. The dewar will have optical windows in the side to allow viewing of the liquid helium in the inner test cell. The data recording is intended to be digital data stored on a hard disk. The float package will be self-contained except for power and supply of liquid helium.

The completed dewar float package will be taken on the DC-9 for one or more flights to observe the motion of the liquid in low gravity. The recorded accelerations will be used as an input to a LMSC-developed CFD code that incorporates the two-fluid model of SFHe. The simulation output will be compared to the actual fluid motion recorded during the DC-9 flight to verify the accuracy of the computer mode.

Task Significance:

The final product of the project will be to have a CFD code for SFHe that has been verified in low gravity. This will allow predictions of SFHe behavior on future satellites such as SIRTF, GP-B, and AXAF with increased confidence in the accuracy of the simulation.

Progress During FY 1996:

Tests:

During this last performance period, considerable progress had been made. The dewar which was shipped to the NASA Jet Propulsion Laboratory (JPL) at the end of October 1995 was integrated into the JPL "Low Temperature Flight Facility". Full-up systems test were performed at JPL prior to shipment of the dewar, the JPL Facility, and the ground support equipment to NASA Lewis. Flights on the aircraft were performed. Two series of tests were performed on the aircraft. The first series of tests was performed to determine if fundamental slosh frequencies could be correctly predicted based on the gravitational field. During these tests, the Float Package which contains the dewar was kept secured to the aircraft. High-gravity data were recorded prior to and after the aircraft descent during the parabolic maneuver.

A series of test were performed at zero-gravity. In these tests the experimental Float Package was allowed to free-float in the aircraft. After entering the zero gravity trajectory, the fluid would transition from a high-g profile to the zero-gravity disc profile. The fluid was then disturbed and the resultant motion recorded.

Tests were conducted in the laboratory at 1-g to measure the SFHe slosh frequency and damping.

Analysis:

It is presently planned to complete the computational analysis of the data taken during the aircraft flights and in the laboratory. The fluid CFD models are being exercised against the data. Two models are being used. The first is a CFD code by FLOWSCIENCE called FLOW3D and the second is a modified version of FLOW3D that incorporates the "two fluid model" aspects of Superfluid helium.

The 1-g simulations are showing that the slosh frequencies and damping coefficients calculations are being predicted

correctly with both models. The interesting results to date has shown that the fluid in 1-g behaves like a Newtonian fluid in respect to slosh frequency and damping. Results of tests show that modeling of SFHe in 1-g can be accomplished with single-fluid models which will accurately predict fundamental frequencies and damping of the fluid motion. Over a range of accelerations where surface tension forces are not dominant, both single and two-fluid models predict fundamental frequencies. This is based on data taken over a range of 0.04 to 2.0 G. Of main interest to designers of spacecraft attitude control systems are frequencies in zero-g. The data recorded during zero-g is still being evaluated, however it appears that durations in aircraft testing may be too short to get conclusive data. The author is evaluating over possible test configurations such as testing with a smaller test cells.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/93 EXPIRATION: 10/96

PROJECT IDENTIFICATION: 962-24-07-18

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Frank, D.J. "Dynamics of superfluid helium in low gravity: A progress report." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA Document D-13845 (1996).

Investigation of Future Microgravity Atomic Clocks

PRINCIPAL INVESTIGATOR: Prof. Kurt Gibble

Yale University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The task is to find a way to build satellite-based laser-cooled atomic clocks capable of 10^{-16} accuracy and 10^{-15} stability for an averaging time of 1 second.

Task Description:

The most important data needed to design a laser-cooled clock is the cold-collision cross-sections. These have not been measured for rubidium (Rb) and cannot be calculated from theory alone. We will first measure the relevant cross-sections for ^{87}Rb and, if these are suitable, we will demonstrate a laser-cooled clock with high stability and accuracy. If the cross-sections will not allow high stability and accuracy, we will measure the corresponding cross sections for ^{85}Rb .

Task Significance:

Measurements of cold-collision cross sections are fundamentally important to establish the theory that is needed for many experiments with cold atoms including Bose-Einstein condensation and better atomic clocks. Developing more accurate atomic clocks is important because they may enable dramatic improvements in interplanetary navigation and potential improvements to the widely used Global Positioning System GPS.

Progress During FY 1996:

Considerable progress has been made in the brief period of FY96 that we were funded on our laser-cooled Rb fountain clock project. With Chad Fertig, a first year graduate student, we've furnished a new lab including a new optical table, we have built two external-cavity diode lasers that are stabilized to Rb transitions, have finished the first stage of the vacuum system assembly and pumped it down to ultra-high vacuum, and we have completed the bulk of the laser work for injecting multiple slave lasers. Recently Wenko Sueptitz, a former Humboldt fellow, has joined our group as a postdoctoral fellow to work on this project. Wenko is well-suited for the project as he has already considerable laser-cooling experience as a HEP Fellow with Wolfgang Ertmer and a DAAD fellow with Phil Gould at the University of Connecticut.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/96 EXPIRATION: 5/98

PROJECT IDENTIFICATION:

NASA CONTRACT No.: NAG3-186

RESPONSIBLE CENTER: JPL

Condensate Fraction in Superfluid Helium Droplets

PRINCIPAL INVESTIGATOR: Prof. J. Woods Halley

University of Minnesota

CO-INVESTIGATORS:

Giese, C.

University of Minnesota

Campbell, C.

University of Minnesota

Goetz, K.

University of Minnesota

Task Objective:

The scientific goal of the proposed project is to obtain information about the condensate fraction in superfluid helium four by studying elastic scattering of helium atoms from a freely floating macroscopic sphere of the fluid.

Task Description:

During the last year we have repeated experiments demonstrating the use of Cs-covered surfaces to partially suspend He for a ground-based experiment and have produced preliminary prototypes of the sources and detectors for the planned transmission experiment. A ^3He - ^4He refrigerator for use in this experiment will be delivered in November 1996.

Our computational studies of various magnetic suspension methods have led to a design of which a prototype has been built using neodymium iron boride magnets. This prototype was used to suspend bismuth. Many-body calculations of transmission rates in the experiment are being carried out numerically by graduate student Arun Setty.

Task Significance:

The condensate fraction of the superfluid helium wavefunction is the microscopic manifestation of Bose condensation which is universally believed to be the origin of the fluid's superfluid properties (as originally proposed by London more than 50 years ago). If successful, the experiment would be important because direct experimental study of the condensate fraction has proved extremely elusive. Only neutron scattering experiments give direct information, and interpretation of these has proved difficult.

Our basic idea is that, in a microgravity environment, it will be possible to do a tunneling experiment (analogous to a Josephson tunneling experiment in some respects) in order to study the condensate. We envision sending pulses of gaseous helium atoms at one side of a suspended sphere of superfluid helium four and detecting helium atoms emerging in coincidence from the other side of the sphere.

Progress During FY 1996:

1. Overview

The objective of this project is the completion of a ground-based study of the scientific and technical feasibility of an experiment in which the presence and nature of the long-range quantum coherence (condensate) in superfluid ^4He is detected. Pulses of gaseous helium will be fired at a suspended droplet of superfluid ^4He and the resulting emission of helium atoms will be detected.

2. Theory

Theoretical results from the previous fiscal years are reported in previous Progress Reports. This work suggested the existence of a large effect but also clarified the need for a more complete many-body analysis of the problem. Analytical aspects of this analysis were completed in the 1994 fiscal year. This year numerical work has continued to make the needed variational calculations with graduate student Arun Setty. We are carrying out variational Monte Carlo calculations of the wave functions describing the reflection and transmission of incident helium particles from a suspended slab such states. The variational wave function for these scattering states depends on 5 parameters: the amplitude and phase of the transmission coefficient, the phase of the

reflected wave, and two parameters characterizing the shape of the envelope of the incoming, reflected, and transmitted helium wave functions. We vary these parameters systematically to bring the following quantities simultaneously as close as possible to their known values: the energy and the values of the current at a set of points inside the slab of superfluid.

The numerical calculation of the current corresponding to this wave function has turned out to be a formidable task. The difficulties include particularly the requirement that the wave function conserve current. Our first attempts at wave function optimization revealed that the first forms used for the variational function lacked sufficient flexibility to satisfy this current conservation requirement. Recent results for the current are much better. Numerical difficulties are also formidable and have been attacked by writing many of the variational expressions in forms which dramatically reduce the number of integrals that need to be calculated by variational many-body methods during a parameter search. We hope to have definitive results from these difficult many-body calculations within a few months.

We have continued to study weak coupling models of the condensated mediated process with NSF sponsored undergraduate research intern Steven Clayton during summer 1996.

3. Suspension of Superfluid with Cesium Surfaces

We are engaged in two types of ground-based experiments. Former NASA Graduate Student Researcher M. C. Williams is carrying out the experiments at Minnesota to demonstrate the feasibility of a method for producing two parallel helium surfaces using the fact that cesium surfaces are not wet by superfluid ^4He . During the past two years, this experiment was successful in demonstrating the possibility of levitating a film of liquid helium in this way. A report of preliminary experiments at temperatures between 1 and 2 K was published in Physical Review B. In these experiments, up to 2 mm of helium was suspended over a 70 micron hole in a cesium-covered platinum disc using this method. A capacitance bridge was used to measure the liquid level. We found that, consistent with theoretical predictions which we made, liquid at depths greater than about 2 mm ran through the hole at velocities consistent with critical velocities reported by others. Suspension using the method was confirmed in more than 6 runs at various temperatures in this range.

In view of the success of this experiment, we are carrying out a version of the experiment for studying the condensate in a configuration in which the superfluid is a suspended slab. A dilution refrigerator has been acquired with funds provided by the University of Minnesota, and was delivered by Janus Instrument Company in October, 1996. The refrigerator has a large working space particularly suitable for the condensate experiment. Installation of the refrigerator in Minnesota should be complete within a few months. It will be used first to test sources and detectors for the production and pulses of helium pulses to be used in the condensate experiment. These sources and detectors are under current development by NASA Graduate Student Researcher Keith Lidke who has been producing and testing zinc bolometers for use as detectors during the last two months. Satisfactory methods for attaching leads to these bolometers have been perfected and measurements of the resistance of the zinc films have been carried out. Design of electronics for the fast detection of incoming pulses is underway and a detecting bolometer should be ready for testing in the dilution refrigerator at about the time that the refrigerator is installed.

4. Magnetic Droplet Suspension

Magnetic suspension has often been suggested as a method for droplet suspension of liquid helium in a microgravity environment. Experiments at Brown University were successful recently in achieving magnetic suspension of helium droplets on Earth using superconducting magnets. As an alternative, NASA Graduate Student Researcher J. Schmidt of this group has carried out a study of the possibility of using permanent magnets for this purpose. If it can be achieved, this method would have great advantages with respect to simplicity and expense. It may even be possible to achieve suspension of helium droplets on Earth using permanent magnets. To study these possibilities, Mr. Schmidt developed computer codes for determining the optimum configuration of permanent magnets, which codes were orders of magnitude more efficient than previously existing software. A permanent magnet configuration was found which produces a field configuration which can suspend helium droplets. It consists of a pie-shaped configuration of magnets arranged so that the magnetization points inward in two dimensions toward a central point. We have shown that the resulting magnetic field configuration should be capable of suspending a small (order of 0.1 mm) superfluid helium droplet. A prototype of this magnet configuration was constructed using neodymium iron boride magnetic material and was used to suspend bismuth

particles during the last year. A study of the dynamics of the suspended particles is under way using video imaging. The next stage in this development, which will require additional funding, is to build a version of this prototype for use in our dilution refrigerator, using Praseodymium Iron Boride material, which has better magnetic properties for our purposes than Neodymium Iron Boride. We have acquired requisite PrFeB material for this project.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 3

TASK INITIATION: 1/93 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-24-07-14

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Williams, M. C., Giese C. F. and Halley, J. W. Suspension of Superfluid Helium Using Cesium-Coated Surfaces. Physical Review B, vol. 53, 6627 (1996).

Proceedings

Halley, J. W. "Progress and Prospects for the 4He Condensate Experiment." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop, NASA Document D-13845 (1996).

Halley, J. W. "Prospects for an Ultralow Pressure Gauge Based on Brownian Motion of a Suspended Particle." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop, NASA Document D-13845 (1996).

Presentations

Halley, J. W. "Computational and Experimental Explorations of the Possibility of Condensate Mediated Absorption and Reemission in Superfluid Helium Four." Workshop on Quantum Evaporation, Pisa, Italy, December 13-17, 1995.

Halley, J. W. "Progress and Prospects for the 4He Condensate Experiment." 1996 NASA/JPL Low Temperature Microgravity Workshop, Pasadena, April 9-11, 1996.

Halley, J.W. "Prospects for an Ultralow Pressure Gauge Based on Brownian Motion of a Suspended Particle." 1996 NASA/JPL Low Temperature Microgravity Workshop, Pasadena, April 9-11, 1996.

Ultra-Precise Measurements with Trapped Atoms in a Microgravity Environment

PRINCIPAL INVESTIGATOR: Dr. Daniel J. Heinzen

University of Texas, Austin

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Our task objectives for FY96 are to observe and study Bose-Einstein condensation, and to confine ultra-cold atoms in a blue-detuned optical dipole force trap. Such ultracold atoms are crucially important for potential zero-gravity applications because they dramatically reduce the required strength of the confining potential. In turn, employing a weaker confining potential reduces the perturbations to atomic transition frequencies introduced by the confinement and should allow for a dramatic increase in resolution and accuracy in atomic resonance experiments. These steps should bring us closer to our ultimate goal of realizing ultraprecise measurements with trapped atoms in a zero-gravity environment.

Task Description:

Bose-Einstein condensation experiments will be carried out in an apparatus designed to produce nanokelvin temperature atoms. In this apparatus, we have recently succeeded in trapping up to 10⁹ rubidium atoms in a magnetic trap, and evaporatively cooling them. In addition to studying the properties of the condensate, we plan to begin experiments designed to demonstrate the possible applications of evaporatively-cooled atoms to a microgravity environment. For example, the atoms will be transferred from the magnetic trap into a blue-detuned optical dipole force trap. The ultralow momentum spread of the evaporatively-cooled atoms will significantly ease the requirements to generate a large-volume optical trap. Such large-volume optical traps would be well suited to spectroscopic applications in a microgravity environment. In a separate apparatus, Zeeman resonance experiments will also be performed with laser-cooled Cesium atoms.

Task Significance:

Precision atomic resonance devices have tremendous practical and scientific importance. An important example is the atomic clock, which has widespread applications to navigation, geophysical measurement, and astrophysics. Precise tests of fundamental scientific principles such as time-reversal symmetry are also carried out with such devices. Substantial advances in the accuracy of these devices are therefore of great importance. One very promising avenue is to make use of ultracold, laser-cooled atoms. These atoms can move as much as 10,000 times more slowly than the atoms in conventional devices. This very low velocity can in principle substantially increase the accuracy of an atomic resonance device. This is because certain measurement errors are proportional to the velocity of the atoms. Unfortunately, gravity seriously limits the usefulness of laser-cooled atoms for this purpose, because it quickly accelerates the atoms back to high velocities. Thus, only in the gravity-free environment of space can the full potential of these ultracold atoms be realized. Our goal is to develop techniques that could be used to produce and store a large number of ultracold atoms in the gravity-free environment of space. If successful, atomic resonance devices based on these techniques could lead to dramatic increases in accuracy.

Progress During FY 1996:

During the past year we have successfully trapped 10⁹ Rubidium atoms in a magnetic trap and evaporatively cooled them, realizing a compression of the phase space density of the atoms by a factor of several hundred. With further work, we should be able to realize temperatures in the nanokelvin range, resulting in Bose-Einstein condensation. We have also rebuilt our Cesium trapping apparatus, resulting in a much longer trap lifetime and improved optical access.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 0

PhD Students: 1

TASK INITIATION: 9/94 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 962-24-08-14

NASA CONTRACT No.: NAG8-109

RESPONSIBLE CENTER: JPL

Precision Measurements with Trapped, Laser-Cooled Atoms in a Microgravity Environment

PRINCIPAL INVESTIGATOR: Dr. Daniel J. Heinzen

University of Texas, Austin

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

New work will be carried out on our two apparatuses. The first apparatus is a magnetic rubidium atom trap, and the second a magnetically-shielded cesium (Cs) atom trap. Our objective for the first apparatus is to demonstrate cooling of atoms to nanokelvin temperatures and to realize Bose-Einstein condensation. Fundamental studies of the condensate will be carried out, including its thermodynamic, optical, and coherence properties. In addition, we plan to transfer the Bose-condensed atoms into an optical trap, which will allow us to trap and to study atoms in arbitrary spin states and to carry out spectroscopic investigations that are not possible in a magnetic trap. Our objective for the second apparatus is to carry out new Zeeman resonance experiments designed to demonstrate "quantum control" of the Cs spin wavefunction. Such control is of fundamental interest, and will allow us to optimize the sensitivity of an electron electric dipole moment search using the Cs Zeeman resonance transitions. In addition, we will continue the development of this apparatus, making additional improvements that will allow us to begin a search for the electron electric dipole moment in subsequent years.

Task Description:

We have recently succeeded in trapping 10⁹ atoms in our rubidium apparatus, and evaporatively cooling them. The atoms were trapped in a quadrupole magnetic trap, and compression in phase space density by a factor of several hundred was realized. We have also installed and tested additional coils to produce a "TOP" trap of the type first demonstrated by Cornell and Wieman at Colorado. The TOP trap overcomes certain limitations of the quadrupole trap, allowing cooling of the atoms to much lower temperatures. Our next step is to transfer the atoms into the TOP, further evaporatively cool them to nanokelvin temperatures, and thus to realize Bose-Einstein condensation. During this first year we will carry out studies of the optical, thermodynamic, and coherence properties of the condensate. We will also attempt to trap the evaporatively-cooled atoms in a blue-detuned far-off resonance optical dipole force trap, using an existing Ti:sapphire laser in our laboratory. We will begin development of a high-power diode laser system to replace the Ti:sapphire laser in subsequent years. This improvement would represent a first step in demonstrating the significance of ultracold atoms for microgravity. Note that the very low momentum spread of the trapped atoms significantly eases the conditions for optical dipole trapping. In our Cs apparatus, we will carry out additional Zeeman resonance experiments designed to demonstrate quantum control of the spin wavefunction. We will also begin four additional improvements in this apparatus: (1) We will go to a "double trap" configuration, in which atoms will be loaded into a high-pressure cell magneto-optical trap, then transferred to a low pressure trap in the experiment region. This process will allow us to obtain a high loading rate and long trap lifetime simultaneously, and will also minimize the magnetic trapping fields needed in the experimental region. (2) We will add electric field plates. (3) We will undertake a dramatic improvement in the magnetic shielding. (4) We will add dipole-force trapping to the apparatus, which will allow us to obtain long confinement and coherence times. We anticipate that these four steps can be 50% completed during FY96. These steps will allow us to undertake a measurement of the electron electric dipole moment in subsequent years that should result in a significant improvement upon the present bound.

Task Significance:

Precision atomic resonance devices have tremendous practical and scientific importance. An important example is the atomic clock, which has widespread applications to navigation, geophysical measurement, and astrophysics. Precise tests of fundamental scientific principles such as relativity are also carried out with such devices. A very significant example is the search for an electron electric dipole moment (edm). Such an edm, if detected, would constitute unambiguous evidence for new physics outside the standard model. For all of these reasons, advances in the accuracy of these devices are therefore of great importance. One very promising avenue is to make use of atoms that have been cooled to ultralow temperatures with laser or evaporative cooling. Laser-cooled atoms can move as much as 10,000 times more slowly than the atoms in conventional devices. Evaporatively cooled atoms can reach even lower temperatures, which for bosonic atoms can lead to Bose-Einstein condensation. Bose-condensed atoms

represent the ultimate in atomic cooling, since such atoms have a momentum spread limited only by quantum mechanics. The velocity spread of such a sample can be less than 10^{-5} m/s. These very low velocities can in principle substantially increase the accuracy of an atomic resonance device. This is because certain measurement errors are proportional to the velocity of the atoms. Unfortunately, gravity seriously limits the usefulness of laser-cooled atoms for this purpose, because it quickly accelerates the atoms back to high velocities. Thus, only in the gravity-free environment of space can the full potential of these ultracold atoms be realized. Our goal is to develop techniques that could be used to produce, store, and spectroscopically probe a large number of ultracold atoms in the gravity-free environment of space. If successful, atomic resonance devices based on these techniques could lead to dramatic increases in accuracy.

Progress During FY 1996:

This task was a new start late in FY96.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-24-04-

NASA CONTRACT No.: NAG3-190

RESPONSIBLE CENTER: JPL

Collisional Frequency Shifts near Zero-Energy Resonance

PRINCIPAL INVESTIGATOR: Prof. Randall G. Hulet

Rice University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The first objective of this project is to measure the collisional frequency shift of the 228 MHz atomic clock transition in ${}^6\text{Li}$. ${}^6\text{Li}$ is expected to have the largest collision frequency shift of any known atomic species at ultralow temperatures.

Task Description:

Since the collisional cross-section is expected to strongly depend on temperature below 1 mK, the realization of the objective requires the capability to laser cool to ultralow temperatures and to measure those temperatures. The atoms are initially confined to a magneto-optical trap at a temperature of ~ 1 mK, and are then laser cooled to ~ 100 micro-K. Their temperature is measured by releasing the atoms and measuring the rate of ballistic expansion of the atomic cloud. The atomic clock transition frequency will be probed during this free expansion, for several different temperatures.

Task Significance:

Collisional frequency shifts are a limiting systematic effect towards the realization of an atomic clock based on laser-cooled atoms. By exploring the dependence of frequency shifts on the atomic interaction potential and on temperature, we can better learn to control them in practical devices. In a later stage of this project, we intend to demonstrate that collisional interactions can be suppressed via a quantum statistical effect.

Progress During FY 1996:

Significant progress has been made during the first 6 months of the grant period. Our first task objective is to measure the collisional frequency shift of ultracold ${}^6\text{Li}$ atoms. We have trapped ${}^6\text{Li}$ atoms in a magneto-optical trap. In order to measure the collisional frequency shift of the ground-state hyperfine transition (i.e. the "clock transition") the temperature of the trapped atoms must be made sufficiently low. We have first implemented a method for accurately measuring the temperature. The ultracold atoms are confined by a magneto-optical trap. To measure the kinetic temperature of the gas, the atoms are released and allowed to expand ballistically. A pulse of near-resonant light causes the atoms to scatter light which is detected by a CCD camera. By fitting the spatial distribution of the atoms as a function of expansion time, the temperature can be found.

We have succeeded in varying the temperature of the gas of the ${}^6\text{Li}$ atoms over a range of 100 μK to 1 μK . The atoms are confined by laser beams in the magneto-optical trap. The atom temperature can be controlled by varying the intensity and the detuning of the trap laser beams. The ability to control temperature is an important step because the collisional cross section varies almost linearly with temperature in this range. Due to the presence of a zero-energy resonance, the elastic cross section is enormous for all temperatures below 10 μK , and increases as the temperature is decreased to 10 μK .

The next step will be to determine the collisional frequency shift by measuring the ground-state hyperfine splitting of the ${}^6\text{Li}$ atom as a function of temperature.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/98

PROJECT IDENTIFICATION: 962-24-0A-

NASA CONTRACT NO.: NAG3-185

RESPONSIBLE CENTER: JPL

Dynamic Measurement Near the Lambda-Point in a Low-g Simulator on the Ground

PRINCIPAL INVESTIGATOR: Dr. Ulf E. Israelsson

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Duncan, R.V.

Sandia National Laboratory

Task Objective:

The objective of this work is to investigate the non-equilibrium behavior of helium very near the lambda point at small values of applied heat current and under effective gravity conditions from 1 g to 0.01 g.

Task Description:

Non-equilibrium conditions will be created by passing a heat current through the sample. An effective low-gravity environment will be created by applying a magnetic field gradient which closely cancels hydrostatic pressure differences in the sample. A custom-made superconducting magnet will be used to produce the highly uniform magnetic field gradient. This magnet will be procured from a magnet winding company and installed in a thermal platform at JPL. Melting curve thermometers, which can operate well in strong magnetic fields, will be used for high resolution thermometry. A vibration-isolated and magnetically shielded helium dewar will be used to cool the thermal platform in order to minimize noise generation and improve the fidelity of the collected data.

The reduced-gravity conditions will enable a test of theoretical predictions of the effect of small heat currents on the nature of the λ -transition and will allow probing of the interface region between co-existing normal and superfluid portions of the fluid. These measurements are not possible to perform in a regular lab environment on the Earth due to the influence of hydrostatic pressure effects and the need to apply large heat currents to overcome hydrostatic effects, tending to perturb the fluid sufficiently to render the measurements questionable. The suppression of the λ -transition due to heat currents will also be investigated at lower values of the heat current than possible in a one-g environment.

Task Significance:

Recent investigations of the influence of an applied heat current on the properties of helium near the superfluid transition have revealed many new phenomena. Agreement with theories based on scaled mean field calculations and dynamic renormalization group calculations is not good. The disagreement may stem from the fact that theories assume zero-gravity conditions, while experiments are performed in a one-g environment. To overcome the influence of gravity on properties near the transition in a heat current, large values of heat current are required which has detrimental effects on the very properties in need of study. It has also been predicted that imposition of a heat current will change the very nature of the lambda-transition from continuous to first order. Investigating these phenomena in a simulated low-gravity environment would enable lower heat currents to be used and would enable observation of phenomena washed out by gravity effects.

Progress During FY 1996:

During the last fiscal year, all of the components for the experiment were integrated and successfully tested at liquid helium temperatures. During this cooldown, a number of important milestones were reached. A magnetic field in excess of what is required to cancel gravity to the 99% level on the ground was successfully trapped in the magnet. All temperature sensors on the apparatus, including the melting curve thermometers, were calibrated. The operation of all sensors were verified to be within specifications even when the high field magnet was energized. In particular, the melting curve thermometers were shown to be unaffected by the extreme magnetic field environment inside the apparatus. Also, a detailed performance study of the melting curve thermometers was completed, demonstrating that the science objectives can be achieved with the current design. We were able to demonstrate a noise level of less than 10nK in a one Hertz bandwidth. Finally, data gathering routines were developed using Labview software and were used to take preliminary thermal conductivity measurements.

Unfortunately, two problems were identified in the initial cooldown. First, there was a small leak into the vacuum area which led to unacceptable variations in the parasitic heat leak into the helium cell. The leak was small enough

to enable us to run the experiment as planned and to develop detailed data-gathering routines which were successfully run, but the science data collected were unacceptable. Second, none of the side wall thermometers were functioning properly. Despite these problems we were able to demonstrate correct behavior of the system using applied heat currents in the 1 -10 $\mu\text{W}/\text{cm}^2$ range. We were successfully able to ramp the top temperature of the cell in a controlled fashion at constant applied heat current such that the cell moved across the entire range of interest, i.e., from initially full of superfluid to full of normal fluid, and back down again.

Following the warm-up of the experiment, we corrected all the problems encountered during the initial cooldown in a satisfactory manner. Currently, the experiment has been successfully cooled down again, and we are in the early phases of preparing to gather useful data.

The modeling effort initiated in FY-94 was also continued. The modeling was extended during the past year to study a wider range of heat currents, from 1 to 30 mW/cm^2 . The model was also extended to study the effect of varying the thermal resistance between the helium in the cell and the temperature controlled top of the cell. Finally, the model was quantitatively compared to physical data taken in Prof. Ahlers' lab. This comparison to physical data showed some discrepancies which can be attributed to the flow of heat through the cell's side walls. During the coming year, we plan to extend the model to include the effect of the side walls.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 12/92 EXPIRATION: 11/95

PROJECT IDENTIFICATION: 962-24-04-09

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Larson, M., Liu, F.-C., and Israelsson, U. E. "Reducing gravity at the superfluid transition in 4He." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13845, 64-65 (1996).

Dynamic Measurements Along the Lambda Line of Helium in a Low-Gravity Simulator on the Ground

PRINCIPAL INVESTIGATOR: Dr. Ulf E. Israelsson

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Larson, M.E.

Jet Propulsion Laboratory (JPL)

Duncan, R.V.

University of New Mexico

Task Objective:**The objectives of this investigation are to:**

A: Measure the non-linear thermal conductivity in the normal fluid immediately above the lambda-line at lower values of heat current than are possible in 1g and compare the results to recent theoretical predictions.

B: Measure the depression of $T_\lambda(P)$ as a function of heat current and pressure away from the end-plates and at lower heat currents than possible in a 1g environment.

C: Investigate the existence of a change in character to a first-order transition at lower heat currents than possible in 1g.

D: Attempt to measure the width of the superfluid/normal interface and study interface dynamics.

Task Description:

We plan to investigate the influence of a heat current on properties very near the lambda line of liquid helium. Studies of this kind have recently received increased experimental and theoretical attention. Measurements up to this point have been limited to a 1g environment, and have primarily been performed at saturated vapor pressure. In contrast, our investigation will perform measurements all the way up to the melting curve in reduced gravity environments down to about 0.001 g.

Traditional ground-based experiments very near the λ -point are limited by gravitationally induced pressure variations in the helium sample. In order to circumvent this difficulty, we have developed a technique which utilizes the diamagnetic properties of liquid helium and a highly specialized magnetic field configuration to minimize these pressure effects. Using a superconducting magnet with a field-field gradient product of 21.0 Tesla²/cm we can oppose gravitationally induced pressure variations over a limited volume in a helium sample down to a level of about 0.01g.

The thermal conductivity cell is composed of two copper end plugs separated by a thin stainless steel wall. The cell has a heater on the bottom and, for most measurements, the temperature of the cell top will be slowly ramped at a controlled rate through the λ -transition from both above and below. Several temperatures in the cell will be monitored using Melting Curve Thermometers with 3 nK resolution. These thermometers are not affected by the large applied magnetic field in the low-gravity simulator. Also, two temperature probes are compressed against the walls of the cell to measure the temperature profile in the helium sample away from end effects.

Task Significance:

We want to extend the range of measurements of the normal fluid conductivity closer to the transition temperature. By being able to approach the transition more closely without entering the two-phase region using our simulator, we expect to be able to observe and to map out the predicted heat current dependence of the normal fluid conductivity in the non-linear region. This would constitute the first real experimental verification of the breakdown of the linear response to an external heat flux resulting in non-ohmic thermal conductivity.

Another focus of our investigations using the low-gravity simulator will be to look more closely at the heat current dependence of the transition temperature. Currently, the experimental observations of this dependence have shown a significantly stronger dependence on the heat current than can be explained within the available theoretical framework. These theories do not include the effects of gravity or vortices. In the low-g simulator we will be able

to use smaller heat currents than those used previously, therefore decreasing both the influence of induced vortices, and the influence of gravity. Hopefully the low-gravity simulator will more closely resemble the idealized system assumed in the theoretical calculations and provide a more thorough test of the predictions.

Also, the low gravity simulator will be used to search for the predicted change in the nature of the lambda transition from second order to first order under the influence of an applied heat current. This first-order effect has not been observed in 1-g ground-based experiments. By virtue of the reduced gravity environment in our cell, we will be able to use lower values of heat current than previous investigations. This would ensure smaller thermal gradients in the normal helium phase which may make the first order effect more easily observable.

By monitoring the temperature of one or both sidewall mounted thermometers as the interface is slowly moving upward in the cell, it may also be possible to deduce the interface width, at least for small values of the heat current where the interface in 0.01g should have a macroscopic width. Numerical calculations of the expected gravity environment in the cell from the measured field profile in the magnet also indicate the possibility of tuning the field in the magnet such that locally the effective gravity environment is even smaller. By optimally tuning the magnet to produce the lowest possible gravity environment right at one of the side wall thermometers and by positioning the interface right at the same location, it may be possible to probe the interface region at fairly high resolution. Possibilities for studying interface dynamics also exist.

Progress During FY 1996:

This task was a new start late in FY96.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 8/96 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 962-24-04-16

RESPONSIBLE CENTER: JPL

Atom Interferometry in a Microgravity Environment

PRINCIPAL INVESTIGATOR: Dr. Mark A. Kasevich

Stanford University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Our scientific objectives are: (1) to develop a rugged laser cooled source of atoms using DBR (distributed Bragg reflector) laser technology; (2) to use this source and these lasers to demonstrate coherent atom wavepacket manipulation techniques; and (3) to incorporate these techniques into an atom interferometer gravity gradiometer. We plan to experimentally study the performance of the prototype device to evaluate the feasibility of a space-based system.

Task Description:

In year one of the grant period we will develop the laser sources and apparatus needed for the proposed experiments. We will employ standard laser cooling and trapping techniques with atomic cesium to create the cold atomic source. Our first experiments, to be carried out near the end of year one, will focus on demonstration and characterization of the proposed coherent atom manipulation techniques. In year two we will demonstrate and characterize an interferometer accelerometer - first in a low sensitivity regime in order to study potential systematic phase shifts and subsequently in a high sensitivity configuration to explore the potential accuracy and resolution of the device. Since vibrational noise will severely hamper the performance of an Earth-bound accelerometer, we will switch to a more complicated gradiometer geometry which is far less sensitive to vibrational noise in the final stages of the proposed work.

Task Significance:

The convergence of recent advances in the field of laser manipulation of atoms with technological developments in the electronics/opto-electronics industry opens the possibility of a new class of experiments involving laser manipulated atoms in a microgravity environment. In the past five years, light-induced forces have been used to cool ensembles of atoms to temperatures below 1 μ K, providing researchers with a novel source of ultra-cold atoms. These laser cooled sources have revolutionized experimental atomic physics and have led to new classes of precision time standards and inertial sensors. Application of these techniques in a microgravity environment could result in robust gravity gradiometers and gyroscopes with sensitivities exceeding current state-of-the-art devices by several orders of magnitude. Such instruments would have important applications in a number of fields. For example, satellite gradiometry studies yield important geophysical data concerning Earth and ocean dynamics. A satellite-borne accelerometer/gravimeter used in conjunction with the GPS system could be used to obtain highly accurate maps of the global Earth gravity field. In addition, techniques developed for satellite interferometer sensors might also have terrestrial applications in, for example, mineral/oil exploration and navigation. Finally, with minor modification, the techniques could be employed to develop atomic standards with unprecedented accuracy.

Progress During FY 1996:

We have continued to develop precision inertial force sensors using atom interference techniques. We have been developing two instruments: a precision gyroscope and a gravity gradiometer.

Gyroscope

We have demonstrated a Sagnac effect atom interferometer gyroscope which uses stimulated Raman transitions to coherently manipulate atomic wavepackets. We have used this gyroscope to measure the Earth's rotation rate, and have measured a short-term stability for rotations of 6×10^{-5} deg/Öhr. This performance is competitive with state-of-the-art optical gyroscopes.

Our approach has been to use stimulated Raman transitions to coherently manipulate a transversely laser cooled atomic beam. In this geometry approximately 107 atoms/sec contribute to the interference signal. We initially prepare atoms into the cesium (Cs) $F = 3$, $m_f = 0$ level, and subsequently subject the atoms to a three pulse

sequence to divide, redirect and finally recombine atomic wavepackets. Interference is manifested through the number of atoms in the $F = 4$, $m_f = 0$ level after the three-pulse sequence. The resulting Sagnac loop has an area of 25 mm². This corresponds to a fringe shift of ~ 8 radians for the Earth's rotation rate $\omega_e = 7 \times 10^{-5}$ rad/sec. Our signal-to-noise ratio was good enough to split the fringe by 1 part in 500 after 1 second of data collection time.

We developed a new laser system to drive the stimulated Raman transitions needed for wavepacket manipulation. This laser system was developed with the aim of creating a system which is robust and reliable enough so as not to limit the long term stability of the gyroscope. Recall that the stimulated Raman method requires two high-power laser beams which differ in frequency by 9.2 GHz, the cesium clock frequency. Our approach has been to derive these two beams from a master diode laser and a high frequency acousto-optic modulator, and then to amplify these two beams using optical injection locking techniques. A key issue is whether the amplification process introduces low frequency phase noise. By driving the Cs clock transition in the classic Ramsey configuration, we characterized the phase noise in the 1 - 100 Hz band, and demonstrated that these sources can be used for precision measurements.

Gravity Gradiometer

We are developing an instrument to measure gravitational gradients at the 10^{-10} sec⁻²/ÖHz level. The instrument uses established light pulse interferometry techniques to measure the relative accelerations of two laser cooled atomic ensembles. In this progress period, we have brought the UHV (ultra-high vacuum) vacuum system and diode laser systems on-line, and optimized the laser cooled atomic source.

The UHV chamber was designed to be non-magnetic, and provide high F-number optical access to the laser cooling region through all viewports. High optical quality, anti-reflection coated, viewports are attached to the system using an indium seal technique. The system reaches a base pressure of $\sim 5 \times 10^{-10}$ torr. A cold finger controls is used to control the Cs-vapor partial pressure.

The trapping and cooling laser systems consist of two distributed Bragg (DBR) laser diodes, each locked to a Cs atomic resonance using a modulation-transfer saturated-absorption technique. Light from one of the lasers is amplified in a third laser diode before being coupled into an optical fiber system. The optical fibers deliver the light to the apparatus. The final beam-shaping optics are mounted directly on the apparatus to ensure a long-term alignment stability. Using this laser system, we have observed a magneto-optic trap in the UHV chamber, and we are currently optimizing both the temperature and the number of atoms in the trap. The Raman laser system (currently being installed) consists of a DBR master laser diode and two high-power slave diodes, a system that is essentially a copy of the one used for the gyroscope.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/94 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 962-24-08-15

NASA CONTRACT NO.: NAG8-108

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Bouyer, P., Gustavson, T., Haritos, K., and Kasevich, M. Microwave signal generation with optical injection locking. Optics Letters, vol. 21, 1502 (1996).

Bouyer, P., Gustavson, T., Haritos, K., and Kasevich, M. Sensing inertial forces with laser manipulated atoms. IEEE/LEOS Newsletter, vol. 9, 22 (1995).

Proceedings

Bouyer, P., Gustavson, T., Haritos, K. G., McGuirk, J., Thompson, M., and Kasevich, M. "Atom interferometer-based navigation systems." Proceedings of the International Symposium for Optics and Defense (1996).

Bouyer, P., Gustavson, T., Haritos, K., McGuirk, J., and Kasevich, M. "Atom interferometry in a microgravity environment." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13845, 146 (1996).

Books

Young, B., Kasevich, M., and Chu, S. "Atom Interferometry." Edited by: Berman, P., Chapter: Precision measurement with light pulse atom interferometers.

Presentations

Kasevich, M. "Precision measurements with atom interferometers." Physics Colloquium, Los Alamos National Laboratory, July 1996.

Kasevich, M. "Rotation measurements with atom interferometer gyroscopes." Workshop on Atom Optics and Interferometry, Cairns, Australia, July 1996.

Kasevich, M. "Precision measurements of inertial forces using atom interferometry." Atomic Physics Seminar, University of Texas, Austin, April 1996.

Kasevich, M. "Measuring inertial forces with precision atom interferometry." Institute of Theoretical Physics Colloquium, Santa Barbara, March 1996.

Kasevich, M. "Using atom interferometers to measure inertial forces: gyroscopes and accelerometers." Atomic Physics Seminar, University of Oregon, Eugene, March 1996.

Static Properties of ^4He in the Presence of a Heat Current in a Low-Gravity Simulator

PRINCIPAL INVESTIGATOR: Dr. Melora E. Larson

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Israelsson, U.E.

Jet Propulsion Laboratory (JPL)

Task Objective:

Perform a comprehensive program to investigate the influence of a heat current on the specific heat of helium-4 along the lambda line.

Task Description:

Use the existing low-gravity simulator at the Jet Propulsion Laboratory to perform measurements on the isobaric thermal expansion coefficient of helium-4 over a range of pressures while passing a heat current through the helium. The thermal expansion data will then be analyzed to give the specific heat.

Task Significance:

It has been theoretically predicted that the specific heat of helium-4 under the influence of a heat current should show a cusp-like divergence as the lambda-line is approached in temperature from below. This divergence has yet to be seen experimentally and would be significantly easier to observe in the reduced gravitational environment provided by the low-gravity simulator.

Progress During FY 1996:

This task was a new start in late FY96. A search for a postdoctoral fellow was undertaken during the past year, and a candidate was selected at the end of FY96. We are currently finalizing the design of the measurement apparatus for performing the thermal expansion measurements on a thermal conductivity cell.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/96 EXPIRATION: 9/99

PROJECT IDENTIFICATION:

RESPONSIBLE CENTER: JPL

Second Sound Measurements near the Tricritical Point in ^3He - ^4He Mixtures

PRINCIPAL INVESTIGATOR: Dr. Melora E. Larson

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Nash, A.E.
Mulders, N.Jet Propulsion Laboratory (JPL)
University of Delaware

Task Objective:

The task objective is to make high resolution measurements on mixtures of ^3He and ^4He to determine the critical exponents at the tricritical point.

Task Description:

A ^3He refrigerator will be procured and equipped with several stages of thermal control. Thin second sound cells with bolometers that will work near 0.8K will be developed. After the equipment and technology has been developed, high resolution second sound measurements will be made in a cell that is also instrumented to perform density and heat capacity measurements.

Task Significance:

This task will improve upon existing measurements at the tricritical point by an order of magnitude. These measurements will then be compared to existing, exact theoretical predictions for any possible discrepancy.

Progress During FY 1996:

This task had a new start late in FY96. Once the funding was in place at JPL, a contract between JPL and the University of Delaware was set up to support our co-investigator, Dr. Mulders, for preliminary design and testing of second sound detectors and densitometers for measurements near the tricritical point. Dr. Mulders began a professorship at the University of Delaware in September. He is in the process of organizing and setting up a new lab. He already has acquired a small ^3He probe that can be used for making quick measurements on potential second sound detectors that work near the tricritical point temperature. Initially, we will focus on determining the best material for use as a second sound detector while also designing the first second sound cell to use for our preliminary measurements.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/96 EXPIRATION: 9/99

PROJECT IDENTIFICATION:

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Mulders, N., Larson, M., and Nash, A. "Experiments near the tricritical point in ^3He - ^4He mixtures." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop, NASA Document D-13845, 83-84 (1996).

Effect of Confinement on Transport Properties by Making use of Helium Near the Lambda Point

PRINCIPAL INVESTIGATOR: Prof. John A. Lipa

Stanford University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this project is to study the effect of confinement on the thermal conductivity of helium near the lambda point. The thermal conductivity is a transport property most readily accessible to precision measurement, allowing the effects of confinement to be quantified. The extent to which the results could be improved in a microgravity environment will also be studied.

Task Description:

Dohm and collaborators have predicted the first-order departures of the thermal conductivity from the bulk behavior as one approaches the lambda point transition in liquid helium. As the transition is approached, the relevant length scale increases dramatically, allowing the effect to be measured in conventional apparatus. Higher order, nonlinear effects are also predicted, but quantitative information is not yet available. We plan to measure these effects for confinement in a parallel plate geometry as a function of plate separation. Earlier measurements indicated that the first-order effect was different from that predicted. This difference needs to be verified, and higher-order contributions need to be explored.

Task Significance:

The results will be used to test the emerging theory of transport properties in confined geometries, which has application to physical and chemical processes near surfaces or in small channels.

Progress During FY 1996:

An apparatus for thermal conductivity measurements near the lambda point of helium with a variable gap is being developed. A cell with a motorized gap adjusting system was developed and tested for uniformity of translation. Unfortunately, the results were below expectations, possibly due to imbalance in the bellows system used to contain the helium sample. The drive mechanism has been redesigned to improve the transmission alignment and new parts are in fabrication.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 9/94 EXPIRATION: 8/96

PROJECT IDENTIFICATION: 962-24-04-14

RESPONSIBLE CENTER: JPL

Red-Shift Test of General Relativity on Space Station Using Superconducting Cavity Oscillators

PRINCIPAL INVESTIGATOR: Prof. John A. Lipa

Stanford University

CO-INVESTIGATORS:

Turneure, J.P.

Stanford University

Buchman, S.

Stanford University

DiPirro, M.J.

Goddard Space Flight Center

Task Objective:

An improved flight prototype superconducting cavity oscillator will be designed and tested at cryogenic temperatures.

Task Description:

Our analysis of the current situation in superconducting cavity oscillator performance is that substantially improved frequency stability could be achieved when the problems described below are solved. The first, gravity sensitivity, can clearly be much reduced by redesign of the existing cavity support system. The second problem, temperature control, can be alleviated by a factor of 10^3 or so, by using advanced technology that has been developed for LPE. The third and fourth areas of improvement involve upgraded electronics. A number of areas of the existing design need attention and the use of modern microwave hardware will be advantageous. Two areas requiring special attention are cavity power control and relative phase measurement. It appears that by using modern technology and servo controls, the former area can be improved substantially. The relative phase measurement between two or more oscillators is the primary output information of interest.

We first planned to develop the details of the circuit design. Critical components will be identified and subjected to analysis. In parallel, long lead time and critical component procurement will be started as soon as appropriate. With the circuit work under way, we will then design the low temperature portion of the apparatus and the cavity support system. This latter task will involve structural modeling and analysis using existing workstations. Cavity components will then be procured and tests run using an existing low temperature system. Cavity Qs and coupling parameters will be measured. Electronics will then be set up to compare cavity frequencies.

Task Significance:

The output from the task should lay the scientific groundwork for the design of a flight instrument.

Progress During FY 1996:

This project received funds in the last two weeks of FY 96. Work in that period was primarily in the areas of planning and preliminary design. A graduate student was identified to work on the improved mechanical design of the cavities.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 0

PhD Students: 1

TASK INITIATION: 9/96 EXPIRATION: 9/98

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NAG3-194

RESPONSIBLE CENTER: JPL

A Renewal Proposal to Study the Effect of Confinement on Transport Properties by Making Use of Helium along the Lambda Line

PRINCIPAL INVESTIGATOR: Prof. John A. Lipa

Stanford University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The goal of the proposed research is to extend the measurements of the confinement effect of the thermal conductivity to higher pressures to observe effects as a function of the strength of the underlying singularity and to determine the universal features of the behavior. To perform the highest quality measurements, the effect should be measured at very long correlation lengths which can be accessed only in space. On the ground, it is possible to work with correlation lengths of up to a few microns. These lengths should allow a complete exploration of the first-order effect and a partial look at the fully developed region. Also, the effects of substrate dependent forces should be small, increasing the validity of future tests of the expected theoretical calculations. We plan to perform the ground-based experiment as a prelude to a later flight experiment which will be optimized to examine the full confinement effect. The experiment should be the first ever to quantify effects that go beyond the first-order boundary effect, for crossover to two dimensions.

Task Description:

After a thermal conductivity cell has been built and operated at the vapor pressure, a new cell will be built for measurements along the lambda line. These cells will be coupled to a high resolution pressure controller capable of operating up to 30 bars. The design of this part of the system will be based on a device currently being built with separate funding in collaboration with JPL. It has a superconducting readout system and a separate forcing coil for pressure adjustment. The main challenge for the new cell design will be how to retain the gap adjustment system and simultaneously operate at high pressures. If necessary, we will design a spring-loaded pressure compensation system to solve this problem.

After the high pressure cells have been constructed, they will be attached to high resolution thermometers and installed in an existing thermal control system. Measurements will be made as a function of temperature at fixed pressure and gap. The data will consist of the temperature drop across a cell as a function of power applied to the bottom heater. From this we will derive the thermal resistance in the limit of small powers.

Task Significance:

The goal of the effort is to improve our understanding of the intrinsic behavior of the thermal conductivity of a fluid very near a wall, but free of substrate effects. Usually, this behavior is impossible to see because the length scale over which it occurs is extremely small: just a few atomic distances. However, the properties of materials in this regime often determine the nature of surface interactions. The measurements will generate new data for comparison with recently developing theories in this area, and also serve as a guide for the design of a possible future flight experiment.

Progress During FY 1996:

Funding for this task was received late in FY '96. Effort to date has focused on developing the high pressure regulation system and on thermometry for the experiment.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 6/98

PROJECT IDENTIFICATION: 962-24-0A-

NASA CONTRACT NO.: NAG3-190

RESPONSIBLE CENTER: JPL

Theoretical Studies of the Lambda Transition of Liquid ^4He

PRINCIPAL INVESTIGATOR: Prof. Efstratios Manousakis

Florida State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

We study the critical properties of liquid helium near the superfluid transition temperature T_λ using recently developed numerical simulation techniques and finite-size scaling. In particular, we are interested in the scaling behavior of the superfluid density and the specific heat. We shall study different finite geometries, namely pure two-dimensional, pure three-dimensional, and the crossover from two-dimensional to three-dimensional superfluidity, in order to verify the validity of scaling and to determine the universal functions associated with scaling.

Task Description:

A recently developed updating technique, called cluster Monte Carlo, which eliminates the long-standing problem of critical-slowing-down will allow us to approach close to the lambda point for large-size lattices and, thus, to extract the critical exponents and scaling properties of the physical quantities of interest. We shall study the temperature and the finite-size dependence of the superfluid density and the specific heat. From these studies we can determine the critical exponent using finite-size scaling techniques.

In addition, we shall determine the superfluid/normal phase boundary $T_\lambda(h)$ for films of thickness h . We shall calculate the superfluid density as a function of the film thickness and we shall examine the validity of the finite-size scaling theory. We shall also calculate the specific heat as a function of h and this will be used to understand the results of the CHeX experiment.

Finally, the role of vortices and the Kosterlitz-Thouless scenario will also be examined in the course of this work. We shall calculate the renormalization group beta function for two-dimensional superfluids and we shall compare it to that predicted by the Kosterlitz-Thouless theory. In addition, we shall study with our simulation technique the intimate connection between the superfluid transition and the unbinding of vortices.

Task Significance:

The results of these studies are relevant and will be compared to the experimental measurements obtained from the lambda-point experiment (LPE) and to the confined helium experiment (CHeX).

Progress During FY 1996:

We studied the specific heat of the x-y model on lattices $L \times L \times H$ with $L \gg H$ (i.e. on lattices representing a film geometry) using the Cluster Monte Carlo method. In the H-direction we applied both periodic boundary conditions and we also used Dirichlet boundary conditions where the order parameter on the top and bottom layers is zero. We find that our results for the specific heat of various thickness size H collapse on the same universal scaling function. The extracted scaling function of the specific heat obtained with Dirichlet boundary conditions is in good agreement with the experimentally determined universal scaling function using no free parameters. This work is published in Phys. Rev. B and in Physical Review Letters.

As an extension of the above simulations we introduced a new model where a Chern-Simons term is coupled to the three-dimensional x-y model. This term endows vortices with an internal angular momentum and thus they acquire arbitrary statistical character. In our interpretation of the Chern-Simons term in the three-dimensional x-y model, it takes an integer value which can be written as a sum over all vortex lines of the product of the vortex charge and the winding number of the internal phase angle along that vortex line. We have used the Monte-Carlo method to study the three-dimensional x-y model with the Chern-Simons term. Our findings suggest that this model belongs to the x-y universality class with the critical temperature growing with increasing internal angular momentum. Applications of this model might be in the area of particle physics or the quantum Hall effect. There are no direct applications for the case of liquid helium. This work is published in Physical Review B.

We also studied numerically the influence of the substrate (boundary conditions) on the finite-size scaling properties of the superfluid density ρ_s in superfluid films of thickness H within the XY model employing the Monte Carlo method. Our results suggest that the jump of the ratio of the superfluid density over the critical temperature at the Kosterlitz-Thouless transition temperature depends on the boundary conditions. This work was published in the Proceedings of the 21st International Conference on Low Temperature Physics.

STUDENTS FUNDED UNDER RESEARCH:				TASK INITIATION: 1/93	EXPIRATION: 12/95
BS Students:	0	BS Degrees:	0	PROJECT IDENTIFICATION: 962-24-07-15	
MS Students:	0	MS Degrees:	0	NASA CONTRACT No.: NAG3-184	
PhD Students:	1	PhD Degrees:	1	RESPONSIBLE CENTER: JPL	

BIBLIOGRAPHIC CITATIONS FOR FY 1996:
Journals

Schultka, N., and Manousakis, E. Specific heat of superfluids near the transition temperature. *Physical Review B*, vol. 52, 7528 (1996).

Schultka, N., and Manousakis, E. Scaling of the specific heat of superfluid films. *Physical Review Letters*, vol. 75, 2710 (1995).

Schultka, N., and Manousakis, E. Three-dimensional X-Y model with a Chern-Simons term. *Physical Review B*, vol. 53, 4782 (1996).

Proceedings

Manousakis, E., and Schultke, N. "Scaling in confined helium: geometry and boundary effects." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13845, 23-27 (1996).

Schultka, N., and Manousakis, E. "Boundary effects on the scaling of the superfluid density." Proceedings of the 21st International Conference on Low Temperature Physics LT-21, *Czechoslovak Journal of Physics*, vol. 46 - Supplement S1, 451 (1996).

Theoretical Studies of Liquid ^4He near the Superfluid Transition

PRINCIPAL INVESTIGATOR: Prof. Efstratios Manousakis

Florida State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

We propose to continue our theoretical studies of liquid helium by applying state of the art simulation and finite-size scaling techniques. We shall calculate universal scaling functions for the specific heat and superfluid density for various confining geometries relevant for experiments such as the confined helium experiment and other ground based studies. In addition, we shall study microscopically the role of the various substrates in imposing a particular boundary condition. Finally, transport coefficients such the thermal conductivity for bulk or confined helium systems will be calculated and their scaling properties shall be determined.

Task Description:

Using Monte Carlo techniques, such as cluster Monte Carlo, which eliminate the long-standing problem of critical-slowing-down, we can approach close to the lambda point for large-size lattices and, thus, extract the critical exponents and scaling properties of the physical quantities of interest. Our previous studies indicate that we can achieve very good agreement with the experimentally determined universal function for the specific heat of confined helium if appropriate boundary conditions are used. From the calculated universal function we can make predictions for the planned confined helium experiment (CHeX).

We plan to continue these calculations in order to obtain more accurate results and even better understanding of the finite-size effects in both the specific heat and superfluid density. Other finite geometries, such as the pore or the droplet geometry will be studied and our universal functions shall be compared to experimental data for the pore geometry.

In addition, we plan to microscopically study the role of the substrates in determining the boundary conditions. For the latter studies, we shall use path integral quantum Monte Carlo methods using the bare helium-helium interaction potential. The role of the substrate in determining the boundary condition on the order parameter and its derivative at the boundary is very important.

In addition, the finite-size scaling and critical exponents of the thermal conductivity of bulk and confined helium shall be studied. For this work we shall use dynamical models, such as the so-called model-F, using real-time evolution of an ensemble of systems at a given temperature and from that we shall extract the appropriate correlation functions.

Task Significance:

The results of these studies are relevant and will be compared to the experimental measurements obtained from the confined helium experiment (CHeX) and several other experimental ground-based studies which are funded by NASA's low temperature microgravity program.

Progress During FY 1996:

We have investigated the scaling of the superfluid density in superfluid films using Dirichlet boundary conditions along the direction of the film-thickness. We studied the scaling of the superfluid density with respect to the film thickness H by simulating the x - y model on films of size $L \times L \times H$ ($L \gg H$) using the cluster Monte Carlo. Periodic boundary conditions were used in the planar (L) directions and Dirichlet boundary conditions along the film thickness. We found that our results can be scaled on a universal curve if we introduce an effective thickness. This is no violation of finite-size scaling since, for much larger size systems than those available to simulations, the effective thickness becomes the true film thickness. In addition, using the same idea we find scaling in the experimental results using the same value of $\nu = 0.6705$. This work has been accepted for publication in the Journal of Low Temperature Physics as a rapid communication.

At the present time we are in the process of completing a more comprehensive numerical study of both the superfluid density and the specific heat of the x-y model on lattices $L \times L \times H$ with $L \gg H$ (i.e. on lattices representing a film geometry) using the Cluster Monte Carlo method. In the H-direction we have applied physical (Dirichlet-like) boundary conditions so that the order parameter in the top and bottom layers is zero, whereas periodic boundary conditions were applied in the L-directions. We find that the system exhibits a Kosterlitz-Thouless phase transition at the H-dependent critical temperature below the critical temperature (λ) of the bulk system. However, right at the critical temperature the ratio of the areal superfluid density to the critical temperature turns out to be H-dependent in the range of film thicknesses considered here. We do not observe finite-size scaling of the superfluid density with respect to H. However, the data can be collapsed onto one universal curve by introducing an effective thickness $H_{\text{eff}} > H$ into the corresponding scaling relations. We argue that the effective thickness depends on the type of boundary conditions. The scaling function f_1 of the specific heat is not very sensitive to this boundary effect within error bars and we find good agreement between f_1 calculated from our Monte Carlo results and the experimentally determined universal scaling function.

We are also in the process of complete an investigation of the scaling properties of the specific heat of the X-Y model on lattices $H \times H \times L$ with $L \gg H$ (i.e. in a pore geometry) with respect to the thickness H, using the 1-Cluster Monte Carlo method. We studied the effect of the geometry and boundary conditions on the shape of the universal scaling function of the specific heat by comparing the scaling functions obtained for cubic, film, and pore geometry. In the presence of physical boundary conditions on the sides of the pore (Dirichlet like), we find good agreement between our Monte Carlo results and experimental data of the specific heat obtained for superfluid helium confined in pores.

The calculations were performed on a heterogeneous environment of computers including Sun, IBM RS/6000 and DEC alpha AXP workstations and a Cray-YMP.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/96 **EXPIRATION:** 4/00

PROJECT IDENTIFICATION: 962-24-0A-

NASA CONTRACT NO.: NAG3-184

RESPONSIBLE CENTER: JPL

Dynamics and Morphology of Superfluid Helium Drops in a Microgravity Environment

PRINCIPAL INVESTIGATOR: Prof. Humphrey J. Maris

Brown University

CO-INVESTIGATORS:

Seidel, G.

Brown University

Task Objective:

The long range goal of our research is the study of the hydrodynamics of drops of superfluid liquid helium by means of microgravity experiments conducted in space. At the present time we are developing a series of earth-based experiments to levitate superfluid drops so that we can acquire data and experience that will be needed for the design of experiments in space.

Task Description:

We are conducting a series of earth-based experiments to study the behavior of superfluid drops. We will develop a means to levitate helium drops in earth gravity, primarily by magnetic levitation. We will then investigate 1) how to inject and position drops in a microgravity chamber, 2) how to manipulate drops and to give them angular momentum, 3) how to observe accurately the vibrations and rotations of the drops, and 4) what drop sizes are best suited for the study of a variety of phenomena.

Task Significance:

The goal is to achieve data and experience critical for the design of experiments in space.

Progress During FY 1996:

We have investigated experimentally methods of simulating microgravity conditions for liquid helium on Earth so as to be better able to design studies of the dynamics of superfluid helium in a microgravity environment in space. We have successfully levitated large drops in a magnetic trap produced by a superconducting magnet. In the process of studying levitated drops in a magnetic trap we observed that two drops in apparent contact often did not coalesce for several minutes. Using a large magnetic field we have stably levitated helium drops of up to 2 centimeters diameter at temperatures down to 1.5 K. To achieve a magnetic force on helium equal to the force of the Earth's gravity requires a product of field times field gradient of 21 Tesla²/cm. A specially-designed superconducting solenoid produces the required field. With the solenoid axis vertical, a stable static trap is created in which helium drops can be levitated indefinitely. Because the trap forces are not spherically symmetric, large liquid drops are substantially deformed. The relative deformation decreases with drop size, falling as the cube of the radius. We have frequently observed two drops in the magnetic trap held in apparent contact for up to 3 minutes without coalescing. This non-coalescence effect is seen only above the superfluid transition temperature. We have been able to explain this effect as resulting from the existence of a vapor layer between the drops caused by evaporation. The evaporation is a consequence of nonequilibrium conditions within the experimental cell such that the drops are slowly cooling by evaporation. Using drops levitated in the magnetic trap we are now in a position to investigate the dynamics and morphology of free superfluid helium drops. The behavior of superfluid drops with angular momentum is expected to be very much different from that of rotating classical fluid drops because, in the superfluid, flow must be irrotational. The experience gained in working with magnetically levitated drops on earth should prove extremely beneficial in the formulation of plans for space-based measurements.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 1/93 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-24-07-16

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Maris, H. J., Weilert, M. A., Whitaker, D. L., and Seidel, G. M. "Magnetic levitation of liquid helium." Proceedings of the 21st International Conference on Low Temperature Physics LT-21 (Prague), Czechoslovak Journal of Physics, vol. 46, Supplement S1, 373 (1996).

Weilert, M. A., Whitaker, D. L., Maris, H. J., and Seidel, G. M. "Magnetic levitation and non-coalescence of helium drops." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop, NASA document, D-13845, 193-195 (1996).

Equilibration in Density and Temperature Near the Liquid-Vapor Critical Point

PRINCIPAL INVESTIGATOR: Prof. Horst Meyer

Duke University

CO-INVESTIGATORS:

Zhong, F.

Duke University

Task Objective:

Ground-based experiments will be carried out to study the density equilibration process at constant average density $\bar{\rho}$ in a pure fluid, (3He), near its liquid-vapor critical point ($T_{c,rc}$) after a step change in temperature ΔT of the container walls. Measurements are to be carried out for both the regions above T_c (one phase) and below T_c (coexisting phases). Numerical simulations are to be performed of the density, temperature and pressure equilibration processes in 3He for the regimes above T_c and below T_c , both ground-based and under reduced gravity. The measurements are to be extended to binary (3He-4He) mixtures near their liquid vapor critical point ("plait point"), and corresponding computer simulations are to be carried out.

Task Description:

Two flat, horizontal cells of somewhat different geometry are used in different series of experiments. The fluid is contained between two parallel flat OFHC copper plates with high thermal conductivity, kept at the same temperature that is regulated to within a few mK before and after the step ΔT . In both cells, the fluid layer height is approximately 4 mm, the diameter is 30 mm and the density is measured by two thin horizontal superposed capacitive sensors, spaced by 2 mm, that record the dielectric constant. The density is then derived via the Clausius-Mossotti relation, and is recorded by both sensors, ρ_{top} and $\rho_{bottom}(t)$, as a function of time t after a programmed small temperature step of the cell walls. At temperatures above T_c , immediately after the step ΔT , the fast density change from adiabatic energy transfer ("piston effect") followed by the slow stratification change at each sensor are recorded by computer. Experiments are carried out along several near-critical isochores and along several isotherms. Below T_c , the two sensors detect respectively the coexisting liquid and vapor phases. The programmed temperature change ΔT in the cell walls will permit following the density evolution in both phases at the sensor locations with time.

With the help of the known scaled expressions for the static and transport properties of 3He above and below T_c , numerical simulations in one dimension are carried out to predict the temporal and spatial evolution of the thermodynamic parameters (density, temperature, pressure and their derivatives) and to predict the asymptotic relaxation times. This simulation is to be done at arbitrary values of the gravitational acceleration g , and will assume the absence of convection - which appears justified by experimental data. The departure from equilibrium values of the properties upon temperature ramping will be investigated by simulation both above and below T_c . Below T_c , the simulations will also predict the motion of the interface between the liquid and vapor phases. After completion of the 3He program, measurements and numerical simulations are to be extended to binary (3He-4He) mixtures.

Task Significance:

Such studies - both for pure fluids and binary mixtures - are very relevant to experiments on fluids under micro-g conditions, where investigations of static and dynamic properties near critical points are to be carried out. It is important to know how long a fluid system takes to approach closely enough thermodynamic equilibrium, and what are the basic mechanisms that control the equilibration process. The numerical computations above T_c are to be compared with experiments. Simulations under microgravity conditions will be able to assess the permissible temperature ramping rate in experimental data taking that will enable measurements of critical properties in a quasi-equilibrium state. In the two-phase regime below T_c , little is known about the equilibration dynamics and the proposed experiments are expected to substantially help in understanding these processes.

Progress During FY 1996:

During this period our projects in conjunction with the investigation of the equilibration dynamics near the liquid-vapor critical point of a pure fluid were as follows :

A) Completion of the paper on the density change and equilibration in ^3He that follows after a small temperature step of the fluid enclosure.

B) Experiments on the density change and equilibration in ^3He along the critical isochore in the regime $T > T_c$ with a new cell of improved design, and analysis of the data and comparison with the computer simulation predictions generated previously.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 1/94 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-24-07-20

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Zhong, F., and Meyer, H. Density equilibration near the liquid-vapor critical point of a pure fluid. II. Coexisting phases for $T < T_c$. Physical Review E, 53, 5935 (1996).

Proceedings

Kogan, A.B., Zhong, F. and Meyer, H. "Dynamics of density equilibration near the liquid-vapor critical point of ^3He ." Proceedings of the 21st International Conference on Low Temperature Physics LT-21 (Prague), Czechoslovak Journal of Physics, vol. 46, Supplement S1 (1996).

Zhong, F. and Meyer, H. "Density equilibration near the liquid-vapor critical point of ^3He II: Coexisting phases $T < T_c$." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop.

Density Equilibration in Fluids near the Liquid-Vapor Critical Point

PRINCIPAL INVESTIGATOR: Prof. Horst Meyer

Duke University

CO-INVESTIGATORS:

Zhong, F.

Duke University

Task Objective:

Ground-based experiments will be carried out to study the density equilibration process at constant average density $\bar{\rho}$ in a pure fluid, (3He), near its liquid-vapor critical point (T_c, ρ_c) after a step change in temperature ΔT of the container walls. Measurements are to be carried out for both the regions above T_c (one phase) and below T_c (coexisting phases). Numerical simulations are to be performed of the density, temperature and pressure equilibration processes in 3He for the regimes above T_c and below T_c , both ground-based and under reduced gravity. The measurements are to be extended to binary (3He-4He) mixtures near their liquid vapor critical point ("plait point"), and corresponding computer simulations are to be carried out.

Task Description:

Two flat, horizontal cells of somewhat different geometry are used in different series of experiments. The fluid is contained between two parallel flat OFHC copper plates with high thermal conductivity, kept at the same temperature that is regulated to within a few millikelvins before and after the step ΔT . In both cells, the fluid layer height is approximately 4 mm, the diameter is 30 mm and the density is measured by two thin horizontal superposed capacitive sensors, spaced by 2 mm, that record the dielectric constant. The density is then derived via the Clausius-Mossotti relation, and is recorded by both sensors, ρ_{top} and $\rho_{bottom}(t)$, as a function of time t after a programmed small temperature step of the cell walls. At temperatures above T_c , immediately after the step ΔT , the fast density change from adiabatic energy transfer ("piston effect") followed by the slow stratification change at each sensor are recorded by computer. Experiments are carried out along several near-critical isochores and along several isotherms. Below T_c , the two sensors detect respectively the coexisting liquid and vapor phases. The programmed temperature change ΔT in the cell walls will permit following the density evolution in both phases at the sensor locations with time. With the help of the known scaled expressions for the static and transport properties of 3He above and below T_c , numerical simulations in one dimension are carried out to predict the temporal and spatial evolution of the thermodynamic parameters (density, temperature, pressure and their derivatives) and to predict the asymptotic relaxation times. This simulation is to be done at arbitrary values of the gravitational acceleration g , and will assume the absence of convection - which appears justified by experimental data. The departure from equilibrium values of the properties upon temperature ramping will be investigated by simulation both above and below T_c . Below T_c , the simulations will also predict the motion of the interface between the liquid and vapor phases. After completion of the 3He program, measurements and numerical simulations are to be extended to binary (3He-4He) mixtures.

Task Significance:

Such studies - both for pure fluids and binary mixtures - are very relevant to experiments on fluids under micro-g conditions, where investigations of static and dynamic properties near critical points are to be carried out. It is important to know how long a fluid system takes to approach closely enough thermodynamic equilibrium, and what are the basic mechanisms that control the equilibration process. The numerical computations above T_c are to be compared with experiments. Simulations under microgravity conditions will be able to assess the permissible temperature ramping rate in experimental data taking that will enable measurements of critical properties in a quasi-equilibrium state. In the two-phase regime below T_c , little is known about the equilibration dynamics and the proposed experiments are expected to substantially help in understanding these processes. The onset of convection near the critical point needs to be understood and our experiments will be compared with hydrodynamic computer simulations.

Progress During FY 1996:

During this period our projects in conjunction with the investigation of the equilibration dynamics near the liquid-vapor critical point of a pure fluid were as follows :

A) Development of a theory for the density response function inside the fluid when the horizontal top and bottom boundaries are subjected to periodic temperature oscillations.

B) Experiments on the fluid density response in the cell at temperatures $T > T_c$ for temperature oscillations of the fluid top and bottom boundaries over a frequency range from 10^{-3} to 5 Hz, analysis of these experiments, and comparison with theory.

C) Preparation of two papers on the theory and experiments of density equilibration in the two-phase region, and of the response of this system when periodic temperature fluctuations are applied as described in item B).

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/96 **EXPIRATION:** 4/00

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NAG3-183

RESPONSIBLE CENTER: JPL

Indium Mono-ion Oscillator II

PRINCIPAL INVESTIGATOR: Prof. Warren Nagourney

University of Washington

CO-INVESTIGATORS:

Dehmelt, H.

University of Washington

Task Objective:

The objective of this project is the development of an ultrahigh resolution optical frequency standard based upon an individual, laser-cooled indium ion. Ultimately, such a standard could have an absolute accuracy of one part in 10^{17} or better (about 4 orders of magnitude better than existing microwave standards). Taking full advantage of the emerging diode laser technology, it should be possible to fit the apparatus into a small package having modest power requirements.

Task Description:

The standard will be based upon an individual, indium ion confined in a radio-frequency trap contained in an ultra-high vacuum enclosure at room temperature. Two ultraviolet laser sources will be provided - each of these will consist of an external cavity infrared diode laser frequency doubled in two steps using nonlinear crystals in enhancement cavities. One laser will cool the ion and detect its presence in the trap. The other will be used for spectroscopy and will be stabilized to a vibrationally isolated optical cavity, ultimately benefiting from the extreme vibrational isolation available in a space-based platform. The latter laser system will eventually be frequency locked to the sharp ion resonance, providing the desired frequency stabilized source.

Task Significance:

An extremely stable optical frequency standard has many possible applications in the areas of metrology, tests of general relativity and the equivalence principle, detection of gravitational waves as well as the more mundane areas of highly precise navigation and surveying. When techniques of precisely relating a microwave standard to an optical one are developed, it will be possible to make an exceptionally accurate time standard based upon a single ion. On the way to these ultimate goals, much new physics can be learned. Examples of the latter are greater insights into the physics of laser cooling and interesting tests of quantum theory involving entangled states and zero-point confinement of single ions.

Progress During FY 1996:

This task was a new start late in FY96.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 7/96 EXPIRATION: 7/00

PROJECT IDENTIFICATION: 962-24-04-

NASA CONTRACT NO.: NAG3-186

RESPONSIBLE CENTER: JPL

Nonlinear Relaxation and Fluctuations in a Non-Equilibrium, Near-Critical Liquid with a Temperature Gradient

PRINCIPAL INVESTIGATOR: Prof. Alexander Z. Patashinski

Northwestern University

CO-INVESTIGATORS:

Ratner, M. A.

Northwestern University

Pines, V.

Case Western Reserve University

Zimmerli, G.A.

New York Military Academy

Meyers, W. V.

Ohio Aerospace Institute

Task Objective:

The objective of this theoretical research is to develop a more complete understanding of the nonlinear behavior of a near-critical liquid in nonequilibrium transient and steady states. The consideration is limited to special physical situations relevant to flight experiments on near-critical fluids. This includes boundary layers and steady states with temperature, density and entropy gradients.

Task Description:

The general theoretical method is the field theory approach to near-critical liquids, the fluctuation theory of critical phenomena, and computer simulations. We study the equilibrium and non-equilibrium long-range correlations in a thin fluid layer near the container wall. Such a layer always occurs in experimental conditions, and the understanding of its contribution is also necessary to correctly interpret the data of past and future light-scattering and other experiments. We study the evolution of a boundary layer following a temperature change on the wall, the fluctuation picture near the wall, and long-range correlations fluctuations in a state with maintained temperature gradients.

Task Significance:

The study of the equilibrium and non-equilibrium fluctuations in an inhomogeneous near-critical liquid is expected to give an insight into phenomena accompanying such changes in experiments very close to the critical point, including already performed flight experiments. The study is expected to yield conditions for achieving a near-critical steady state with a constant heat current and to formulate optimal conditions for a potential flight experiment.

Progress During FY 1996:

We studied the hydrodynamics of adiabatic cooling in a system with a temperature gradient, and estimated the conditions in which the super-heat transfer state may appear in microgravity experiments. In the local equilibrium approximation which is valid at small heat currents, the heat current does not alter the fluctuations on scales smaller than the correlation radius. At larger heat transfers, the heat current becomes the dominant characteristic to determine the correlation radius of density fluctuations. This leads to a new nonlinear heat transfer kinetics, where the dependence of the thermal conductivity on heat transfer become the dominant source of non-linearity. We now analyze the set of heat transfer equations with such a non-linearity.

Fluctuations in an equilibrium boundary layer in a near-critical liquid near a wall are studied using the renormalization group method. The fluctuation characteristics are altered by the wall in a layer of a correlation radius width. During the period covered by this grant, we have studied the boundary conditions on the wall, and generalized the ϵ -expansion technique to include the plain boundary geometry. The wall influence alters significantly the fluctuation in a layer of the correlation radius width. So far, the case of non-absorbing wall has been considered. The study of a wall with adsorption/desorption potential is in progress.

We studied, using computer simulations, the fluctuations of structural characteristics of the liquid. These short-scale characteristics are not included in the conventional theory. The major concern here is the suggested interaction of the local structural order with the critical mode. The possibility to describe the local structural order is studied. The order parameter is found to be a high-rank tensor.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 8/96 EXPIRATION: 7/00

PROJECT IDENTIFICATION: 962-24-04-

NASA CONTRACT NO.: NAG3-193

RESPONSIBLE CENTER: JPL

Superfluid Density of Confined ^4He near T_λ

PRINCIPAL INVESTIGATOR: Dr. David Pearson

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Chui, T.

Jet Propulsion Laboratory (JPL)

Tonucci, R.J.

Naval Research Laboratory

Lipa, J.

Stanford University

Task Objective:

We intend to exploit recent technological advances to extend and to improve Helmholtz resonator measurements of the superfluid density in liquid helium confined to one-dimensional channels, and to study the dissipation of flow in this helium. Utilizing a SQUID-based pressure transducer, nanochannel glass for the confinement medium, and high resolution paramagnetic salt thermometers will allow us to improve the tests substantially on several fronts.

Task Description:

We shall employ a SQUID-based pressure transducer to improve the sensitivity to pressure changes by several orders of magnitude. The improved sensitivity for detecting the oscillatory motions in the Helmholtz resonator will permit a closer approach to the lambda transition, and it will allow us to study the dissipation in more detail.

We shall also use nanochannel glass (NCG) medium to confine the liquid helium. This glass material, developed initially by one of the co-investigators (RJT), contains a regular array of small channels, with the smallest size available in different samples near 17 nanometers. As well, the pore diameters in NCG are uniform to 1%, more than an order better than previous media. Thus we shall employ a state-of-the-art confinement medium to provide better resolution in the measurements.

The high resolution thermometers (HRTs) will be used to control the helium temperature, employing a heater and a servo system. The precise temperature control is required to reduce vapor pressure variations to levels below the resolution of the pressure sensor. These thermometers were developed by two of the co-investigators (JL and TC).

Task Significance:

These results will complement the heat capacity data of the Confined Helium Experiment that is planned for flight on the Space Shuttle late in 1977. As explained above, the measurements will improve the resolution of these data by several orders of magnitude. The combination of critical parameters from the superfluid density data and the critical parameters from the CHeX experiment can be used to test scaling relations.

Progress During FY 1996:

This task was started late in FY96.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 8/96 EXPIRATION: 7/98

PROJECT IDENTIFICATION: 962-24-04-19

RESPONSIBLE CENTER: JPL

Finite Size Effects near the Liquid-Gas Critical Point of ^3He

PRINCIPAL INVESTIGATOR: Dr. Joseph Rudnick

University of California, Los Angeles

CO-INVESTIGATORS:

Barmatz, M.B.
Dohm, V.

Jet Propulsion Laboratory (JPL)
Technische Hochschule Aachen, Germany

Task Objective:

The objective of this task is to begin study of the effects of boundary conditions on the critical point properties of a system in a confined geometry.

Task Description:

The key elements of the theoretical study are associated with the behavior of a system in the universality class of the liquid-vapor system in the immediate neighborhood of the bulk critical point when the system is confined in the sort of container that will be utilized in Earth-bound and microgravity environments. Of special interest to us are the effects of boundary conditions that reflect the real interactions that take place between the liquid-vapor system and the walls of the container. We will perform calculations in which a range of boundary conditions apply. The ultimate goal is the prediction of the temperature and pressure dependence of two key quantities: the isothermal compressibility and the specific heat at constant volume. The problems of immediate interest are how the boundary affects the density (or the order parameter) in its immediate vicinity, how the effects of the boundary extend into the system and how standard methods for the calculation of critical point properties will be affected by boundary conditions.

The main goals of the project in FY96 are:

1. To calculate the position dependence of the order parameter profile in the presence of a variety of boundary conditions.
2. To set up the Renormalization Group in the proper way.
3. To properly formulate the summation over modes that is central to the field-theoretical approach to critical phenomena.

Task Significance:

The significance of the task is twofold: First, it advances our theoretical understanding of critical phenomena, and in particular, of finite size effects near critical points. Second it contributes to the theoretical support of possible future microgravity experiments now being evaluated.

Progress During FY 1996:

The key elements of the theoretical study are associated with the behavior of a system in the universality class of the liquid-vapor system in the immediate neighborhood of the bulk critical point when the system is confined in the sort of container that will be utilized in Earth-bound and microgravity environments. Of special interest to us are the effects of boundary conditions that reflect the real interactions that take place between the liquid-vapor system and the walls of the container. We will perform calculations in which a range of boundary conditions apply. The ultimate goal is the prediction of the temperature and pressure dependence of two key quantities: the isothermal compressibility and the specific heat at constant volume. The problems of immediate interest are how the boundary affects the density (or the order parameter) in its immediate vicinity, how the effects of the boundary extend into the system and how standard methods for the calculation of critical point properties will be affected by boundary conditions.

The project is a new start for fiscal 1996, so nothing has reached the stage of publication as yet. However, a calculation leading to predictions for the behavior of both the susceptibility and the specific heat is now nearing

completion. This calculation assesses the effect of "mixed" boundary conditions on these quantities in the vicinity of the bulk critical point. Of immediate interest are the leading finite-size corrections, as these are the effects likely to be detectable in experiments now being contemplated. Our calculations have resulted in explicit predictions for the magnitude of these leading-order corrections, and we expect to be able to produce results for the behavior of key thermodynamic quantities throughout the finite-size regime.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-24-04-

NASA CONTRACT No.: NAG3-186

RESPONSIBLE CENTER: JPL

Dynamics and Morphology of Superfluid Helium Drops in a Microgravity Environment

PRINCIPAL INVESTIGATOR: Prof. George M. Seidel

Brown University

CO-INVESTIGATORS:

Maris, H.J.

Brown University

Task Objective:

The long-range goal of our research is the study of the hydrodynamics of drops of superfluid liquid helium by means of microgravity experiments conducted in space. At the present time we are developing a series of earth-based experiments involving the levitation of superfluid drops so that we can acquire the data and experience that will be needed for the design of experiments in space.

Task Description:

We are conducting a series of earth based experiments to study the behavior of superfluid drops. We have developed a means to levitate helium drops in earth gravity by magnetic levitation. We shall now investigate how to manipulate drops and how to give them angular momentum. We shall determine how to observe accurately the vibrations and rotations of the drops and how to determine what drop sizes are best suited for the study of a variety of phenomena in space.

Task Significance:

The goal is to achieve data and experience critical for the design of experiments in space.

Progress During FY 1996:

We have investigated experimentally methods of simulating microgravity conditions for liquid helium on earth so as to be better able to design studies of the dynamics of superfluid helium in a microgravity environment in space. We have successfully levitated large drops in a magnetic trap produced by a superconducting magnet. In the process of studying levitated drops in a magnetic trap we observed that two drops in apparent contact often did not coalesce for several minutes. Using a large magnetic field we have stably levitated helium drops of up to 2 cm diameter at temperatures down to 1.5 K. To achieve a magnetic force on helium equal to the force of the earth's gravity requires a product of field times field gradient of $21.5 \text{ Tesla}^2/\text{cm}$. A specially-designed superconducting solenoid produces the required field. With the solenoidal axis vertical, a stable static trap is created in which helium drops can be levitated indefinitely. Because the trap forces are not spherically symmetric, large liquid drops are substantially deformed. The relative deformation decreases with drop size, falling as the cube of the radius. We have frequently observed two drops in the magnetic trap held in apparent contact for up to 3 minutes without coalescing. This non-coalescence effect is seen only above the superfluid transition temperature. We have been able to explain this effect as resulting from the existence of a vapor layer between the drops caused by evaporation. The evaporation is a consequence of non-equilibrium conditions within the experimental cell such that the drops are slowly cooling by evaporation. Using drops levitated in the magnetic trap we are now in a position to investigate the dynamics and morphology of free superfluid helium drops. The behavior of superfluid drops with angular momentum is expected to be very much different from that of rotating classical fluid drops because in superfluid flow must be irrotational. The experience gained in working with magnetically levitated drops on earth should prove extremely beneficial in the formulation of plans for space-based measurements.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	1
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	0

TASK INITIATION: 7/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NAG3-192

RESPONSIBLE CENTER: JPL

Precise Measurements of the Density and Thermal Expansion of ^4He Near the Lambda Transition

PRINCIPAL INVESTIGATOR: Dr. Donald M. Strayer

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Chui, T.

Jet Propulsion Laboratory (JPL)

Yeh, N.-C.

California Institute of Technology

Lysek, M.

Jet Propulsion Laboratory (JPL)

Task Objective:

The objective of this ground-based Annual NRA project is to demonstrate the value of high-precision density measurements in the study of the lambda transition of liquid helium. During the two years of Annual NRA funding, we shall demonstrate the capability to perform high-precision density measurements using superconducting cavities, applying high resolution thermometers (HRTs) for temperature control. We shall also demonstrate the ability to deconvolve nonuniformities caused by gravity from the density data.

Task Description:

We shall employ superconducting microwave cavities having Q-value: near 10^9 , operated in modes that have standing wave patterns that are axially symmetric and whose z-dependences are well known. Upon filling the cavity with liquid helium, and adjusting the temperature near to T_λ , measurements of the cavity resonant frequency will reflect the helium density. Very near the transition a normal-superfluid interface will form in the cavity. Moving this interface across antinodes of the standing wave pattern by high resolution temperature control will allow the density to be probed in the interfacial region. Measurements at many temperatures will provide density data for deconvolving the temperature dependence of the density from the gravity-induced effects.

Task Significance:

We expect that our earth-bound measurements will demonstrate the value of precision density measurements to exploration of the lambda transition, and to study of cooperative transitions in general. The preliminary measurements to be conducted in this Annual NRA task will provide useful information about future exploration of related experiments to be conducted in the microgravity experiments. The results will lead to applications of the technique to problems that include studies at many pressures, studies of nonequilibrium effects, or studies in confined geometries.

Progress During FY 1996:

This task has continued to develop the apparatus for measuring the density of liquid helium using a superconducting cavity, with the goal of deriving the anomalous thermal expansion coefficient near the lambda transition. The fabrication and testing of superconducting cavities have brought us closer to a finished cryoprobe for these measurements. The analysis and modeling of our apparatus have provided assurance that the measurements will provide a precise test of theories of the superfluid transition.

Cavity Tests

We began testing the TM_{010} niobium cavity that was obtained from John Turneaure of Stanford. The precise resonant frequency for the cavity was not known, and how well the cavity stood up to 20 years of sitting on the shelf was also a mystery. Using computer programs written to find and characterize resonant modes, and confining the frequencies to the range for which these cavities were designed, we searched for the high-Q resonance we knew the cavity to have displayed in its earlier life. We were never successful in finding that mode, however, so we concluded that the Q has likely degraded to the point that the fixed coupling to the cavity is insufficient to excite and sense the resonance. Therefore we fabricated our own niobium cavity.

The cavity we designed utilized the TE_{011} modes to obtain the cylindrical symmetry in the electric field that would allow our deconvolution scheme to be applied. We decided that we could work for the first year with somewhat lower Q-values than the 10^9 that we shall eventually seek for work at the lambda transition. So, instead of applying a long-term anneal in high vacuum to the niobium material, we merely anodized the surface to make it

nonconducting and to protect the superconducting layer beneath the anodization. Other workers have reported obtaining Q-values over 10^9 in such cavities at temperatures near 1.0 K. We will be able to prove our techniques with Q-values of 10^8 or greater near T_λ , so we felt such a fabrication method would suit our needs.

We are now testing the cavity for Q and frequency versus temperature behavior. The resonances are found almost exactly where we designed them to be. So far the Q-values have been below our goals.

At the same time, our stable temperature platform has neared completion. The assembly of the parts fabricated last year has progressed to the point of beginning vacuum testing, first at room temperature, and soon at lower temperatures. An injury to the technician who was performing the assembly has caused some delay, but this setback is now righted, with new progress again underway.

Analysis

Our analysis of the technique we have described for deconvoluting the gravity gradients with many measurements of density with the superfluid-normal fluid interface at different positions in the cavity has proceeded over the past year, leading to the reports listed in the bibliography. We conclude that the high precision of the measurements of the cavity frequency will allow us to determine the density and the expansion coefficient to parts in 10^{10} on Earth, and at least 100 times better in space. The limitation on Earth is the stability of the temperature, since the temperature establishes where the interface sits in the cavity. Because we would improve the frequency stability and measurement precision for a space-flight experiment, again the temperature resolution and control will limit the precision of the values of the expansion coefficient that can be derived from the density data. With these high-precision capabilities, we have proposed and won funding for further investigations to develop these techniques, aiming at testing universality in pressurized pure ^4He or in varying mixtures of ^3He - ^4He , and at studying the interface region.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/94 EXPIRATION: 8/96

PROJECT IDENTIFICATION: 962-24-04-12

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Yeh, N.-C., Jiang, W., Strayer, D. M., and Asplund, N. N. "Precise measurements of the density and critical phenomena near the phase transitions in helium using high-Q niobium microwave cavities." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13845, 98-99 (1996).

Yeh, N.-C., Jiang, W., Strayer, D. M., and Asplund, N. N. "Precise measurements of the density and critical phenomena near the phase transitions in helium using high-Q niobium microwave cavities." Proceedings of the 21st International Low temperature Physics Conference LT-21 (Prague), Czechoslovak Journal of Physics, vol. 46, Supplement S1, 181-2 (1996).

Presentations

Strayer, D. M., Jiang, W., Yeh, N.-C., and Asplund, N. N. "Precision density measurements near the helium lambda transition using high-Q microwave cavities." 1996 March Meeting of the American Physical Society, St. Louis, March 20-24, 1996.

Precise Measurements of the Density and Critical Phenomena of Helium near Phase Transitions

PRINCIPAL INVESTIGATOR: Dr. Donald M. Strayer

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Yeh, N.-C.

California Institute of Technology

Lysek, M.J.

Jet Propulsion Laboratory (JPL)

Chui, T.C.

Jet Propulsion Laboratory (JPL)

Task Objective:

The objective of this ground-based research project is to demonstrate the value of high-precision density measurements in the study of the lambda transition of liquid helium. During the previous two years of Annual NRA funding, we demonstrated by analysis the capability to perform high-precision density measurements using superconducting cavities, when high-resolution thermometers (HRTs) are used for temperature control. We have also shown the ability to deconvolve nonuniformities caused by gravity from the density data. With this new grant we shall expand our goals to study liquid helium under different applied pressures, and to study various mixtures of ^3He and ^4He , applying the high-precision density measurements to test predictions of universality at the lambda transition. Another objective is to cool mixtures of the appropriate concentration down to near the tricritical point to test the predictions for the density in the region where the lambda transition and the phase separation curve approach each other.

Task Description:

We shall employ superconducting microwave cavities having Q-values of 109 near T_λ , operated in modes that have standing wave patterns that are axially symmetric and whose z-dependences are well known. Upon filling the cavity with liquid helium, and adjusting the temperature near to T_λ , measurements of the cavity resonant frequency will reflect the helium density. Very near the transition a normal-superfluid interface will form in the cavity: Moving this interface across antinodes of the standing wave pattern by high resolution temperature control will allow the density to be probed in the interfacial region. Measurements at many temperatures will provide density data for deconvolving the temperature dependence of the density from the gravity-induced effects; the precise temperature control required will be obtained by applying paramagnetic salt thermometers to measurement and control of the temperature. As well, a column of liquid helium will be used to apply pressures up to 200 Pascals to test universality of the critical parameters; a capacitive level-measuring device will determine the height of the helium column very precisely, to parts in 10⁸ or better. To prepare mixtures of ^3He and ^4He , and to improve the purity of ^4He samples, we shall apply the "heat-flush" method of adjusting the ^3He concentration as demonstrated by the McClintock group at the University of Lancaster.

Task Significance:

The high precision of the measurements of density will allow new tests of the theories of phase transitions to be performed. To date, most measurements have concentrated on finding a , the exponent in the leading term in the expression for the temperature dependence of the thermal expansion or specific heat, e.g., the thermal expansion coefficient b as given by $b = -1/(dr/dT) = (A/a)|e|^{-a}(1 + D|e|b + \dots)$, where e is the reduced temperature $e = (T - T_\lambda)/T_\lambda$ expressing the closeness to the transition. The very precise density measurements we intend, to parts in 10¹⁰ on Earth and parts in 10¹² in orbit, will permit a and the amplitudes to be measured to approximately parts in 10⁸, in itself an improved test of theory. Such a precision will also enable us to determine accurately the confluent terms D and b in the expression for the thermal expansion coefficient, thereby testing the theories in new ways. This precision will permit quality tests of theory further from the transition than less precise measurements would allow. As well, the precision will enable careful tests of universality of the critical parameters to be performed, either with application of pressure, or with mixing of ^3He into the ^4He sample. The resolution of the paramagnetic salt thermometry will enable the measurements to be carried out over several ($e = 10^{-2}$ to 10^{-7} , at least) decades of the reduced temperature, again improving the test of theories.

Progress During FY 1996:

During the few months that this new task has been funded, we have concentrated on establishing the measurement system. The high-Q niobium cavity has been tested, and is being cleaned and modified slightly in attempts to improve the result. A bakable vacuum system has been procured for annealing the niobium cavity at pressures near 10^{-10} torr while maintaining its temperature in the 1500-2000 C range for periods of a week or longer. The high resolution paramagnetic salt thermometer is built and ready to be installed in the liquid helium can. The capacitive level probe and its oscillator circuit are designed, and parts are being fabricated for its assembly. A few weeks of adding these parts to the cryoprobe will bring us to low temperature tests of the vacuum integrity of the system, followed soon thereafter by real data.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 0

TASK INITIATION: 8/96 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 962-24-04-20

RESPONSIBLE CENTER: JPL

Analysis of Residual Acceleration Effects on Transport and Segregation During Directional Solidification of Tin-Bismuth in the MEPHISTO Furnace Facility

PRINCIPAL INVESTIGATOR: Prof. J. Iwan D. Alexander

University of Alabama, Huntsville

Co-INVESTIGATORS:

Favier, J.-J.

Centre d'Etudes Nucleaire de Grenoble, France

Gerandet, J.-P.

Centre d'Etudes Nucleaire de Grenoble, France

Task Objective:

To determine the effects of well-defined and well-characterized g-jitter disturbances the transport conditions (and effects of residual acceleration) during the plane-front directional solidification of a tin-bismuth alloy under low gravity conditions using a combination of numerical simulation and flight experiments.

Task Description:

The work involves using a combination of 2- and 3-D numerical models, scaling analyses, 1D models and the results of ground-based and low-gravity experiments. The experiments were conducted in the MEPHISTO furnace facility during the USMP-3 spaceflight which took place earlier this year (February 22 through March 6, 1996). Real-time Seebeck voltage variations across a Sn-Bi melt during directional solidification in MEPHISTO on USMP-1 showed a distinct variation which can be correlated with thruster firings. The Seebeck voltage measurement is related to the response of the instantaneous average melt composition at the melt-solid interface. This permitted a direct comparison of numerical simulations (and acceleration data) with the Seebeck signals obtained on USMP-1. Motivated by the results of the comparison we used numerical simulations to predict the response of the Seebeck signal to composition changes at the interface caused by convective disturbances produced by thruster firings of various magnitudes and durations. These simulations were carried out for different solidification rates. The results of the simulations were used to plan a subset of the USMP-3 MEPHISTO experiments dedicated to the evaluation of g-jitter effects. There were several differences between the USMP-3 experiments as compared to USMP-1. Firstly, a more concentrated alloy was solidified on USMP-3, and, secondly, Primary Reaction Control System (PRCS) thruster burns were requested at particular times during four separate growth runs. This allowed us to monitor the Seebeck signal response under well-characterized growth conditions. This allowed for quantification of the effects of "g-jitter" on convective-diffusive transport in the melt through the real-time changes in average interfacial composition obtained from the Seebeck measurement. In addition, guided by SAMS acceleration data, we carried out simulations during the experiment in order to obtain a better comparison of predicted responses with the actual Seebeck signal.

Task Significance:

While there has been much attention focused on g-jitter effects on low gravity experimentation, quantitative experimental data is in most cases lacking. These experiments represent the first attempt to quantitative correlation between well-characterized residual accelerations and the response of an actual experimental solidification system. The results will be invaluable to future experimenters and facility designers planning for operations on the space station.

Progress During FY 1996:

The experiments were conducted in the MEPHISTO furnace facility during the USMP-3 spaceflight which took place earlier this year (February 22 through March 6, 1996). The first quantitative experimental results concerning the effects of microgravity disturbances on the directional solidification were obtained. Comparison of the real-time (raw, uncorrected) Seebeck signals with the predicted Seebeck signal calculated from the evolution of the simulated composition profiles showed excellent agreement.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 0

TASK INITIATION: 5/95 EXPIRATION: 4/96

PROJECT IDENTIFICATION: YOF2248

NASA CONTRACT No.: NAG3-174

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Alexander, J.I.D., Scaling and estimation of experiment response to g-jitter. Microgravity Quarterly, vol. 5, (November 1, 1995).

Garandet, J.P., Corre, S., Gavaille, S., Favier, J.J., and Alexander, J.I.D., On the effect of gravity perturbations on composition profiles during Bridgman crystal growth in space. J. Crystal Growth, (1996).

Proceedings

Alexander, J.I.D., "Response of crystal growth experiments to time-dependent residual acceleration." Proceedings of the 9th European Symposium on Gravity Dependent Phenomena in Physical Sciences, vol. 464, eds. L. Ratke, H. Walter and B. Feuerbacher (Springer Verlag, Berlin) 95-105, 1996.

Presentations

Alexander, J.I.D., "Quantitative experimental characterization of g-jitter effects on directional solidification." presented at the 31st Annual COSPAR meeting, Birmingham, England, July 14-21, 1996.

Synthesis and Characterization of Single Macromolecules: Mechanistic Studies of Crystallization and Aggregation

PRINCIPAL INVESTIGATOR: Dr. Spiro D. Alexandratos

University of Tennessee, Knoxville

CO-INVESTIGATORS:

Cook, K.

University of Tennessee

Joy, D.

University of Tennessee

Phillips, P.

University of Tennessee

Wunderlich, B.

University of Tennessee

Task Objective:

The principal objective is to prepare single-molecule polymer amorphous particles and crystals by thermally induced precipitation/crystallization from bulk dilute solutions and by precipitation/crystallization via solvent evaporation from electrosprayed nanodroplets of dilute solutions. Polymer-polymer interactions will be controlled in order to compare the effects of interchain and intrachain entanglements on the chemical and physical properties of a polymer particle or crystal. Successful preliminary studies will be extended to studies in microgravity which will allow for a much more sensitive probing of intermolecular interactions through differences in properties of the polymers.

Task Description:

An electrospray attachment will be constructed for a conventional mass spectrometer, allowing for individual polymer chains to be isolated as they emerge from the instrument. Gravity complicates their isolation but its effect could be minimized with very dilute solutions. The morphology of the single chains will be characterized by high resolution low voltage scanning electron microscopy. Backscattered electron imaging will also be utilized, with spatial resolution of 1-3 nm. Thermal analysis will reveal details of chain motion, including details of crystallization kinetics and the effects of inter- and intrachain entanglement.

Task Significance:

The commercial and technological importance of plastics cannot be overstated. Specially designed plastics have been applied as materials in aerospace construction, medical prosthetics, and organic semiconductors. This wide range of applications stems from the wide diversity of chemical and physical properties of the macromolecules (i.e., polymers) which serve as the building blocks of the plastics we encounter. While our understanding of the origins of this diversity has advanced in recent years, it remains far from perfect. With the increasing importance of composite materials, the gap between theory and experiment may even be widening. An investigation into the role of the interactions between discrete macromolecules on the final observed macroproperties requires the availability of samples of controlled molecularity (i.e., one, two, three, ... macromolecules). It is the goal of this research to prepare and characterize samples comprised of single polymer molecules of known molecular weight, then compare the observed properties with those of comparably well-controlled systems where the number of interacting macromolecules is known. This will allow for the design of new plastics with targeted properties including strength, durability, and biodegradability.

Progress During FY 1996:

The feasibility of isolating single-chain molecules was established experimentally by electrospraying amorphous polystyrene. An optimization of the process discussed in the FY95 progress summary enabled the consistent production of single-chain particles. A bimodal size distribution was found representing the size of single-chain particles and larger, few-chain clusters. Tailoring of the spraying conditions enables the production of different sizes of the few-chain cluster. Therefore we were able to produce distinct particles with predominantly 1, 10 or 100 polymer chains for example. In this manner one can fill the gap between single-chain particles and bulk material. The particles were observed and the corresponding number of polymer chains was derived. The imaging was done with atomic force and scanning electron microscopies. Further work to scale-up the technique and produce larger amounts of particles for macroscopic investigation is in progress. Spraying of a crystalline polymer, poly(ethylene oxide), lead to single crystals with different numbers of chains. Because of the limited chain number, those crystals enable the detailed study of crystallization and backfolding processes. Preliminary annealing experiments suggest a

decreased melting temperature due to the finite size. Finally, small emulsion polymerized latex particles were used to evaluate coalescence and the specific glass transition temperature of the particles by differential scanning calorimetry.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/94 **EXPIRATION:** 11/96

PROJECT IDENTIFICATION: 962-21-08-25

NASA CONTRACT NO.: NAG8-106

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Festag, R., Alexandratos, S.D., Cook, K.D., Joy, D.C., Phillips, P.J., and Wunderlich, B. "Synthesis and characterization of single macromolecules: Mechanistic studies of crystallization and aggregation." Microgravity Materials Science Conference, Report Summaries Volume, 24-25 (1996).

Festag, R., Wunderlich, B., Joy, D.C., Alexandratos, S.D., and Cook, K.D. "Separation and characterization of single-chain polymer particles (in "Space Processing of Materials," N. Ramachandran, ed.)." Proceedings of SPIE 2809, 155-165 (1996).

Presentations

Cook, K.D., Festag, R., Wunderlich, B., Joy, D.C., and Alexandratos, S.D. "Separation and characterization of single-chain polymer particles." SPIE Annual Meeting, Denver, Colorado, August 4-8, 1996.

Festag, R., Alexandratos, S.D., Cook, K.D., Joy, D.C., Phillips, P.J., and Wunderlich, B. "Synthesis and characterization of single macromolecules: Mechanistic studies of crystallization and aggregation." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Festag, R., Wunderlich, B., Alexandratos, S.D., and Cook, K.D. "Separation and Characterization of Single-Chain Polymer Particles." American Physical Society, March Meeting, St. Louis, Missouri, March 18-22, 1996.

Microgravity Impregnation of Fiber Preforms

PRINCIPAL INVESTIGATOR: Dr. M. C. Altan

University of Oklahoma

CO-INVESTIGATORS:

Lai, F.C.

University of Oklahoma

Kline, R.A.

University of Oklahoma

O'Rear, E.A.

University of Oklahoma

Grady, B.P.

University of Oklahoma

Task Objective:

The objective of the proposed research is to contribute to the understanding of microgravity impregnation and wetting of isotropic and anisotropic porous media, and to develop low-pressure molding methodologies to fabricate high-performance composite materials which cannot be realized on earth. Investigating the effects of capillary forces and gravity on resin transfer mold filling will be among the primary objectives. The flow through porous media induced during the filling of a center-gated mold cavity will be studied under microgravity conditions. The proposed experiments aim at understanding the effects of fluid viscosity, external pressure (i.e., impregnation pressure), surface tension, and microstructure of the wetted porous media on the flow kinematics and impregnation quality.

Task Description:

The proposed study involves experimental and theoretical investigation of impregnation of a porous medium placed in a thin gapwidth, diverging planar cavity. In particular, the radially diverging flow and spreading of a Newtonian and a viscoelastic thermosetting resin through: i) ceramic porous media; and, ii) glass fiber preforms will be studied. These materials are used most often to fabricate high-performance molded parts and are particularly suitable for lightweight space structures. In addition, the possibility of utilizing a surface modification process invented at the University of Oklahoma to facilitate wetting of the ceramic porous media and fibrous preforms with an organic resin will be investigated. Real-time diagnostics for the bulk flow behavior and the spatial formation of macro- and microvoids will be accomplished by optical means as well as piezoelectric transducers. In the case of impregnation by an organic resin, the effect of microgravity on the fiber/resin interface and adhesion quality will be analyzed at micron and submicron levels with an Atomic Force Microscopy (AFM) and a Small Angle X-ray Scattering System (SAXS) after the resin is fully cured.

Task Significance:

It is now well-known that the spreading of liquids and wetting of solid surfaces in space exhibit a number of significant fluid management challenges as well as numerous interesting phenomena. Many of these phenomena are also technologically important in fabricating high-performance parts in space such as the structural components needed to build the space station or similar large space platforms. The ability to manufacture geometrically complex, lightweight and high-performance composite parts in space primarily depends on understanding and subsequent controlling of flow processes such as filling a mold cavity, spreading or coating a solid surface, and impregnation of a porous fiber preform. For example, most high-performance molding operations involve impregnation of a fibrous preform where the balance between viscous and surface forces as well as nonisothermal effects significantly affect the fluid behavior. It is believed that microgravity provides the necessary means to mold much stronger/stiffer composite materials due to achieving higher volume content of the reinforcing preform with less defects such as voids and dry areas. In addition, the complete process can be accomplished with much simpler, lighter, and inexpensive tooling and molding equipment.

Progress During FY 1996:

It has been five months since we started the project "Microgravity Impregnation of Fiber Preforms." During the initial stages of the project, we emphasized the design and assembly of the experimental set up; acquisition of the necessary equipment; formulation of theoretical research and identification of important parameters; and graduate student recruitment.

The initial design of the experimental molding set up is now complete. With this experimental molding set up 1-g and microgravity experiments will be carried out. The mold cavity has a circular shape with a radius of 9 inches. We designed the mold to have the flexibility of changing the gap width of the cavity by using different aluminum spacer plates. Thus, we will be able to experiment with 1/4, 3/8, and 1/2 inches wide cavity thicknesses. The circular inlet gate is located at the center of the cavity with an inlet diameter ranging from 1/4 to 1/2 inches. The overall mold dimension is 20 x 20 inches, and assembled by 20 uniformly spaced 1/4-inch bolts. We designed the mold to work as a closed-loop system where the injection fluid is circulated via a high precision peristaltic pump. In order to eliminate the injection pulsations an on-line pulse dampener is used. The pump head is selected to yield a flow rate of 200-8000 ml/min. This should be adequate to fill the mold within seconds and capture the details of the flow kinematics under microgravity conditions. With this design we have the capability to control the injection volume flow rate via the data acquisition system. The viscosity limits are decided to be between 50 to 2000 cp. In the first phase of experiments corn syrup is diluted with water to achieve different viscosity levels. The bottom mold wall is designed to have four pressure transducers arranged along a radial line to capture the pressure field during the filling. The pressure transducers have a range of 0-100 psig with a 0.3% accuracy. They also have 500G shock resistance. We have designed a new probe to determine the fluid front shape as the fluid progresses in the mold cavity. Based on the total electrical resistance of the fluid in between two parallel probes one can obtain information about the local interface shape. This method will also give us information about the degree of cure of the thermosetting resin after the fluid front has passed the probes.

The mold is designed to be used with the Omega portable data acquisition system with a sampling rate up to 100,000 samples per second. The interface cards are acquired for the pressure transducers, thermocouples, and interface probes. The injection flow rate is also controlled by this system. The complete data acquisition system is hooked up to a personal computer or to a lap top via a PCMCIA interface.

On the theoretical front, we started to develop the numerical code to simulate filling of a mold cavity. Preliminary analysis of the important parameters showed that for our set up, the ratio of Bond number to Capillary number changes from approximately 0.1 to 1000 in the microgravity and 1-g conditions, respectively. In both cases, Reynolds number may be less than 1. After a critical review of the literature, it has been decided that a finite element method with a predictor-corrector scheme is the appropriate choice to determine the transient location and the shape of the fluid interface as well as the flow kinematics throughout the cavity. The developed code will be first validated by the available steady solutions and the experimental data. Then, it will be applied to a horizontal two-dimensional rectangular and disk-shaped cavity.

The fiber wetting and surface modification component of the project is being carried out under the direction of co-principal investigators Ed O'Rear and Brian Grady. A systematic search was carried out to track down possible suppliers of a single fiber tensiometer. This device will be used to measure wetting properties or, more specifically, the contact angle between the fiber or modified fiber and resin. Prospective units were identified from two separate manufacturers. The unit selected offered an order of magnitude greater sensitivity, computer-control and data acquisition, and other added capabilities at a slightly higher cost. The fiber tensiometer has been received, set up and tested. A recent software upgrade for the unit has been installed.

Our graduate student recruitment efforts for this project have been very successful. Two students are currently supported in the School of Aerospace and Mechanical Engineering. Chien-Te Li, a Ph.D. student, was recruited to work on theoretical analysis and numerical modeling issues. Kristian A. Olivero will start his graduate studies in the Spring 1997 semester to pursue a Ph.D. degree in Mechanical Engineering; he will be primarily involved in the molding experiments and data analysis. In addition, two chemical engineering graduate students have recently been recruited to work on the project. After presentations and the formal administrative procedure, both Brian Sweeney and Michael Hwa listed the "Microgravity Impregnation of Fibers" project as their first choice for thesis research. A graduate of West Virginia Tech, Brian will be working for a master's degree while Michael from University of California-Davis aims to obtain a Ph.D. Since the grant provided funding for only one student in this area, Drs. Grady and O'Rear decided to provide supplemental funding to support an additional student. It is believed that the scope of the project could provide sufficient work for two students. Thus, we are pleased to convey that the University of Oklahoma will be picking up the additional uncommitted match to the NASA grant in the form of a research assistantship.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1

MS Students: 1

PhD Students: 2

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-21-45

NASA CONTRACT NO.: NAG8-127

RESPONSIBLE CENTER: MSFC

An Electrochemical Method to Visualize Flow and Measure Diffusivity in Liquid Metals

PRINCIPAL INVESTIGATOR: Dr. Timothy J. Anderson

University of Florida

CO-INVESTIGATORS:

Narayanan, R.
Fripp, A.L.University of Florida
NASA Langley Research Center (LaRC)

Task Objective:

The objective of this research program is to develop solid state electrochemical titration procedures to identify the dynamic convective states in liquid metals that can occur when the liquid metal sample is subjected to density gradients. Density gradients in liquid metal processing are produced by solutal or thermal gradients and can sufficiently influence processed material properties. An important aspect of the general objective is to assess the effect of geometry on the convective state. Central to the microgravity application of the technique is knowledge of the oxygen diffusivity in liquid metals since the diffusive velocity is comparable to the convective velocity. An ancillary objective is then to measure oxygen diffusivities without data corruption by convective effects and to understand the constitutional relationships.

Task Description:

To define the limits of the technique, ampoules of different geometrical cross section will be constructed with electrochemical sensors located along the ampoule walls. Oxygen will be titrated into or out of the liquid metal and the diffusivity of oxygen will be determined. Simultaneously the measurements taken at the sensing cells will determine the dynamic state of the liquid metal. The deduced dynamic state will be compared with a numerical model that represents the essential features of the physics of the problem. To better understand the correct temperature dependence of the oxygen diffusivity, molecular dynamic simulation will be performed.

Task Significance:

Identification of the fluid flow state is important in a number of materials processes including crystal growth from the melt. This technique will not only provide benchmark values of the diffusivity of oxygen in liquid metals but also will provide direct measurement of the convective states of a liquid metal process. It is anticipated that this technique will be useful in defining flow states in a microgravity environment and thus assist in the interpretation of microgravity experiments. Furthermore, ground-based experiments on model geometries will add to the experimental knowledge base in the field of fluid physics and provide data for numerical model verification. Finally, it is envisioned that this tool can be applied to the control of liquid metal processes.

Progress During FY 1996:

During the first three months of this project substantial progress has been made in constructing an ampoule with a rectangular geometry. The purpose of titration and sensing experiments with this geometry is to test the predicted flow patterns in a well posed geometric configuration and thereby "calibrate" the flow sensor. 3-D calculations are in progress and the model has been checked against theoretical asymptotic limits.

STUDENTS FUNDED UNDER RESEARCH:BS Students: 1
MS Students: 1
PhD Students: 0

TASK INITIATION: 7/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-21-33

NASA CONTRACT NO.: NAG8-124

RESPONSIBLE CENTER: MSFC

A Novel Electrochemical Method for Flow Visualization

PRINCIPAL INVESTIGATOR: Dr. Timothy J. Anderson

University of Florida

CO-INVESTIGATORS:

Narayanan, R.

University of Florida

Fripp, A.L.

NASA Langley Research Center (LaRC)

Task Objective:

The objective of this research program is to develop and demonstrate a novel electrochemical technique to visualize the dynamic states in high temperature liquid metals. This technique uses the oxygen anion-conducting ceramic electrolyte yttria stabilized zirconia as a crucible material which holds a model liquid metal (tin) in a Bridgman configuration. Electrochemical cells will be constructed at various positions along the side wall and bottom of the solid electrolyte. The bottom cell will operate in the electrolytic mode to establish a well defined boundary condition with respect to the titrated oxygen tracer concentration. The side wall cells will be operated in the galvanic mode to measure the dynamic oxygen concentration at the various wall locations. Well defined convective flow patterns will be established for this model geometry and the results will be compared to numerical predictions of the flow patterns. In this manner the sensitivity of the technique will be determined.

Task Description:

In order to identify the sensitivity of the technique, a cylindrical crucible with local electrochemical cells at 5 vertical and 4 azimuthal positions (20 total cells) will be constructed. The flow directions of dynamic states (oscillatory flow) developed in a Sn melt in a destabilizing vertical temperature gradient will be studied. In this experiment, a single cell will be electrochemically pulsed and the time response monitored at the other cells. The experiment will be repeated with different electrolytic cells and pulsing experiments will also be performed to identify the natural oscillation frequency. In a final series of experiments, the continuous response of the sensor cells will be measured to a step change in boundary condition. The results will be compared to a complete 3-D calculation of buoyancy-driven flow accounting for sidewall conduction and radial transport.

Task Significance:

In the processing of many advanced materials (e.g., the bulk crystal growth of semiconductors) the fluid flow state of the liquid determines the quality of the material produced. Although flows in the liquid are not intentionally created, natural forces produce flows. Since the melt is often at high temperature, exhibits a high vapor pressure, and is opaque, it is extremely difficult to visualize the fluid flow pattern. Thus, one must rely on the results of calculations and their associated uncertainties. A novel method is being developed to measure flow patterns in liquid metals by using solid state electrochemical sensors to measure the time variation of a tracer species. In a microgravity environment, it is anticipated that the magnitude of natural fluid flow will be greatly reduced and produce improved materials. In order to correlate material properties to the fluid flow pattern, we must know the pattern. This technique promises to provide such insight. Potentially, the method could be adapted for improved process control and manufacturability.

Progress During FY 1996:

A modified Bridgman ampoule, constructed from recrystallized alumina incorporated with multiple electrochemical sensors (YSZ plugs), was used to visualize the convective flow patterns in high temperature liquid metals.

Dissolved oxygen was used as the tracer species, which could be potentiostatically injected or extracted locally at one of the sensors and the oxygen concentration changes were monitored at the other cell locations on the melt/electrolyte boundary in the galvanic mode as a function of time. Flow patterns were inferred for different aspect ratios of the melt and as a function of the imposed temperature gradient. The technique was also able to discern transcritical points in the dynamic states of the melt.

Computer-based data acquisition of the temperature and voltage readings was possible by interfacing the electrochemical cells with a PC carrying a DAS-1600 card.

We intend to test this flow visualization technique in a low gravity environment. It is essential to isolate the diffusion component from the convective component, both of which are comparable in a microgravity environment. Therefore an electrochemical cell was specifically designed to measure the molecular diffusivity of oxygen across cylindrical tin melts, prior to flow visualization studies.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	2	BS Degrees:	1
MS Students:	1	MS Degrees:	0
PhD Students:	0	PhD Degrees:	0

TASK INITIATION: 7/94 EXPIRATION: 7/96

PROJECT IDENTIFICATION: 962-21-08-26

NASA CONTRACT No.: NCC8-051

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Prasad, S., Mallika, C., Narayanan, R., and Anderson, T.J. "A Novel Flow Visualization Technique for the Determination of Dynamic States in a Bridgman Crystal Growth Configuration." AIAA 96-0255, 34th AIAA National Meeting.

Presentations

Anderson, T.J., and Narayanan, R. "A Novel Electrochemical Method for Flow Visualization." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Mallika, C., Narayanan, R., and Anderson, T.J. "Modeling of Fluid Flow Occurring During the Measurement of Diffusivity in Liquid Metals." Second Fluids in Space Conference, Naples, Italy, May 1996.

The Effects of Convection on Morphological Stability during Coupled Growth in Immiscible Systems

PRINCIPAL INVESTIGATOR: Dr. J. B. Andrews

University of Alabama, Birmingham

CO-INVESTIGATORS:

Coriell, S.

National Institute of Standards and Technology (NIST)

Task Objective:

This study is designed to investigate the influence of convection on morphological stability of the solid-liquid interface during directional solidification in immiscible systems. Ground-based experimentation has revealed that variations in microstructure may occur as a result of fluid flow at the solid-liquid interface. In some cases this flow may even be capable of disrupting the coupled growth process necessary for the development of desired fibrous microstructures.

This study will combine observations made utilizing transparent metal-analog systems with a detailed analysis of fluid flow on a microscopic and macroscopic scale. The first step will involve a theoretical analysis to determine the anticipated fluid flow at the solidification front. The analysis will then move into a combined experimental/theoretical stage where experimentation will be carried out to either verify or disclose weakness in the theoretical portion of the analysis. The findings will make a significant contribution to a better understanding of the role of fluid flow on steady state solidification and coupled growth in immiscible alloys.

Task Description:

This investigation will start with modeling of the density variations in the liquid adjacent to the solidification front. The density variation due to the thermal and solutal fields will be calculated to determine the magnitude of the buoyancy force involved with each. Anticipated flows resulting from the above density variations will then be calculated and experimentation will be carried out to verify the model.

A transparent metal-model system will be utilized in order to facilitate flow visualization. The very small cell wall spacings to be used initially in this study (10 μm) will result in significant damping of buoyancy driven fluid flow. This damping may be sufficient to result in convective stability for very thin sample cells. The sample cell thickness will be varied in order to control fluid velocities ahead of the solidification front. Cell spacings from 10 μm to 1.0 mm will be utilized in order to vary the flow velocities. Non-reactive tracer particles will be utilized to track flow patterns that develop in the cells and to determine flow velocities.

Task Significance:

The significance of this project lies in the knowledge to be gained on the influence of fluid flow on processes at the solidification front and the structures obtained during directional solidification of immiscible alloys. Under the proper processing conditions fibrous microstructures can be produced which may make some immiscible alloys useful as advanced superconductors or magnetic materials. However, flows which occur naturally during processing these alloys influence the stability of the fibrous growth process and negatively impact the ability to form desired structures. The findings from this study will result in a dramatic improvement in the level of understanding of the interactive processes controlling fibrous growth in these immiscible systems.

Progress During FY 1996:

Work on this new project has only been underway for a short time period. One of the first tasks has involved the modification of a temperature gradient stage microscope for use with a new sample configuration for this investigation. This work primarily requires changes which will allow observation of the solidification front during vertically upward growth. This work is currently in progress.

In the modeling area, preliminary work has begun on the variations in density in the liquid ahead of the solidification front to allow flow velocity calculations. To date this work has focused on variations due to the composition field. The influence of the temperature field will follow.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 1

TASK INITIATION: 4/96 **EXPIRATION:** 4/00

PROJECT IDENTIFICATION: 962-21-01

NASA CONTRACT No.: NAG8-122

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Andrews, B., and Coriell, S. "The Effect of Convection on Morphological Stability During Coupled Growth in Immiscible Systems." Extended Abstract, Microgravity Materials Science Conference, Report Summaries Volume, 32-33, 1996.

Presentations

Andrews, B., and Coriell, S. "The Effect of Convection on Morphological Stability During Coupled Growth in Immiscible Systems." Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.

Foam Metallic Glasses

PRINCIPAL INVESTIGATOR: Prof. Robert E. Apfel

Yale University

CO-INVESTIGATORS:

Li, W.

Yale University

Task Objective:

The original scientific objective was to determine the parameter space for which foamed glasses are possible. This objective has been expanded to include foamed polymers created by the process of dynamic decompression and cooling. The engineering objectives are to design apparatus to operate in this parameter space and to investigate the practicality and desirability of this process for satisfying technological needs and for producing new opportunities for the application of these materials.

Task Description:

Amorphous materials are an important class of materials because of their many unique features, such as the absence of crystal defects (e.g., grain boundaries or dislocations) and a wide compositional range over which a single-phase amorphous material can be formed. A novel processing approach and experimental design to achieve as-cast bulk amorphous materials are investigated, since a bulk form of amorphous material is required in many applications. By sudden decompression of a melt that is seeded with a volatile liquid, the dispersed "foaming" liquid vaporizes, taking its latent heat of vaporization from the melt, thereby homogeneously cooling the melt. Due to a high decompression rate, a sufficient cooling rate may be produced to yield an amorphous solid foam.

The experimental program is divided into three major sections: (1) proof of foaming principle with organic materials; (2) tests with the water-tin system, even though it is known that such systems will not form a glass; and, (3) tests of alloy and organic polymer system for forming a foamed metallic glass. The first of these is to verify our expectations with regard to the foaming process and the production of a bulk foam. The second is to give us experience with a metallic system that others have worked with and which may present behaviors unique to metals and not observed with organic materials. The third step is obviously an important milestone toward foamed metallic glasses and/or foamed polymers. The experimental program will be complemented by a theoretical/computational study of this highly transient "foaming" process and by comprehensive materials analysis of all product specimens.

Task Significance:

Rapid decompression of seeded melts, or "dynamic decompression and cooling (DDC)" is a novel processing approach to producing amorphous foam materials, which is an open solid bulk structure that may have glass properties and low density. Foam metallic glass and organic polymer materials should possess few structural defects and may have many potential applications, such as lightweight and high strength structural materials, or matrix materials that can be filled with other materials to suit some special requirements.

Progress During FY 1996:

Our most recent work has focused on polymers. Experimental work has proceeded with poly(butylene terephthalate) (PBT) and polyethylene, and with a variety of blowing materials.

We have begun with PBT because it has become an important engineering thermoplastic polyester for many applications requiring good solvent resistance, mechanical properties, dimensional stability, and good processability. It has a relatively high crystallinity (60%), which is hard to suppress by conventional cooling methods even though it has a glass transition temperature above room temperature ($T_g = 67^{\circ}\text{C}$). High crystallinity means relatively low impact resistance and toughness, which excludes PBT from some important applications, such as automobile body panels.

The premise here is that if we can produce a PBT polymer with significantly greater amorphous phase, we can improve the impact resistance. Moreover, if the structure of the polymer includes a significant component of

amorphous fibers, then the resulting foam product may have strength to weight ratios better than those found in traditional foaming processes.

SPECIFIC DATA:

The primary assessments made of our DDC samples have been:

1. Average density of the foam: Foams with densities of 10-15% of the original PBT materials have been produced.
2. Electron micrographs: Show a variety of foam structures with fibers and granules; foam structure is more irregular (perhaps fractal?) than traditional foams. SEM images permit detailed view of a variety of microstructures.
3. Tensile testing: Exhibits two stages of stress increasing with strain, and failure as a ductile material (passing through a yield point before failure). Failure strain is higher than for normal polymer foams when stretching below T_g.

APPLICATIONS:

Among the possibilities for applications are: light-weight engineering structural materials with or without sandwich structure, epoxied filled composites, catalyst support, filter, insulator, special packaging, *et al.*

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 3/93 EXPIRATION: 12/96

PROJECT IDENTIFICATION: 962-25-08-24

NASA CONTRACT No.: NAG8-947

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Apfel, R., and Qui, N. Principle of dynamic decompression and cooling for materials processing. vol. 11, (1996).

Qui, N., and Apfel, R. Rapid decompression of seeded melts for materials processing. Rev. Sci. Instrum., vol. 65, 3337-3343 (1995).

Ostwald Ripening of Liquid and Solid Droplets in Liquid Metal Matrices

PRINCIPAL INVESTIGATOR: Dr. Alan J. Ardell

University of California, Los Angeles

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to investigate the influence of volume fraction, f , on the kinetics of Ostwald ripening (coarsening) of either liquid or solid "droplets" in a liquid metal matrix, and to compare the data with the predictions of existing theories, especially in the regime of very small volume fractions (< 0.05). It is proposed to achieve this objective by continuously monitoring the variation of electrical resistivity, ρ , of the liquid matrix caused by the depletion of solute concentration, C , that inevitably accompanies the growth of the droplets. Unlike prior research on this problem, the proposed experiments do not involve measurements of particle sizes and size distributions, hence the attendant difficulties of quenching of the alloys from the liquid state and uncertainties associated with preservation of the liquid-state "microstructure" are avoided. Calculations of ρ for two-phase mixtures show that when f is small all changes in ρ can be attributed to changes in C , since the contribution of the dispersed droplets to ρ is negligible.

Task Description:

The initial task is to design and construct the circuitry required to measure changes in electrical resistivity in the neighborhood of 10^{-3} to 10^{-2} n Ω ·m (1 n Ω ·m = 0.1 $\mu\Omega$ ·cm). Theoretical estimates indicate that the expected changes in C during coarsening, which produce these small variations in ρ will be in the range of parts per million. The measurement of such small changes in resistivity poses a difficult challenge, especially *in-situ* at the temperatures of the experiments, but changes in ρ smaller than 10^{-3} to 10^{-2} n Ω ·m have been detected using circuits reported in the literature. It is intended to make these measurements using a contactless method employing a sensitive bridge circuit. Proof of concept will be demonstrated by experiments conducted using solid specimens. Subsequently, experiments will be performed using candidate liquid alloys (e.g., Zn-Pb) chosen so that f is relatively small.

Task Significance:

Theories that predict the rate at which a physical process occurs in liquids are often very difficult to test using liquid specimens. Ostwald ripening, which involves the rate at which small particles or "droplets" suspended in the liquid grow to larger sizes, is representative. Ripening is inevitable because energy is associated with the interface between the small particles and the liquid in which they are suspended. Reduction in the area of the interfaces lowers the internal energy of the system, and therefore drives the ripening phenomenon. An analogous process is the elimination of small bubbles as a froth coarsens, eliminating the energy of the membranes separating the gas in the bubbles. In Ostwald ripening the small solid or liquid droplets have densities that differ from that of the suspending liquid. This causes settling or buoyancy in a terrestrial environment, and collisions among the droplets that adversely influence the kinetics of true ripening. A microgravity environment is therefore essential for successfully conducting experiments on ripening in liquids. A thorough understanding of ripening is important because of its relationship to the stability of arrays of nanometer size particles in solids. Systems containing particle arrays of this type are potentially important in ground-breaking new engineering structural, electronic and optical materials applications.

Progress During FY 1996:

During the initial four months of this program, we have concentrated our efforts on the design and construct of a sensitive bridge circuit which must be capable of measuring very small changes in electrical resistivity (10^{-3} to 10^{-2} n Ω ·m). Our approach involves contactless measurement of resistivity using the change in mutual inductance of coaxially wound coils, consistent with published circuits. A sensitive lock-in amplifier has been purchased for detecting the small changes in mutual induction that obtain when the concentration of solute in the matrix changes with aging time during coarsening. Mutual induction coils have been wound, and experiments are in progress to optimize the geometry that provides the highest sensitivity. A novel aspect of the design of the entire experimental

apparatus is the attempt to include a small furnace inside the coils, so that the coils themselves will not be subjected to a fluctuating temperature environment. The heating elements of the furnace, which will initially be nichrome wire, will be parallel to the axis of the mutual induction coils, and will in principle not affect the measurements. Water cooling between the heating elements and the coils will ensure that the coils do not heat up during an aging experiment. Preliminary work indicates that the power requirement for the furnace in this arrangement is not exceptional. Temperature control is intended to be maintained through the use of a regulated DC current supply, and temperature gradients will be eliminated through combinations of element winding geometry and heating of independent elements, strategically situated along the length of the furnace.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 2
PhD Students: 0

TASK INITIATION: 6/96 EXPIRATION: 6/98

PROJECT IDENTIFICATION: 962-21-02

NASA CONTRACT NO.: NAG8-123

RESPONSIBLE CENTER: MSFC

Nucleation and Cluster Formation in Levitated Droplets

PRINCIPAL INVESTIGATOR: Prof. Stephen Arnold

Polytechnic University, New York

CO-INVESTIGATORS:

Izmailov, A.F.

Polytechnic University, New York

Myerson, A.S.

Polytechnic University, New York

Task Objective:

1. Employment and improvement of the existing experimental Electrodynamic Levitator Trap (ELT) technique in order to investigate stochastic motion of the ELT confined microdroplets of supersaturated solutions in the case where the dimensionless drag a and driving b parameters are much greater than one.
2. Development of an appropriate theoretical formalism to describe stochastic motion of the ELT confined microdroplets of supersaturated solutions in an atmosphere near the Standard Temperature and Pressure for the case where the dimensionless drag a and driving b parameters are not necessarily small (less than one).

Task Description:

Components of this research include:

1. Experimental study of stochastic motion of the confined levitated microdroplets of various supersaturated solutions. The containerless levitation allows one to considerably delay nucleation onset and, thus, provides a unique method to study the formation and evolution of subcritical solute clusters. This study includes measurement of such time-dependent microparticle characteristics as the standard deviation of its confined stochastic motion, activity of the solute dissolved, etc. Since the measured characteristics are extremely sensitive to the appearance of subcritical solute clusters (solid inclusions) inside of the studied microdroplet the proposed experiment provides an unique opportunity to study the metastable state of matter.
2. Development of theoretical models of the microparticle confined stochastic motion for the two principally different cases: (1) when there are no solid inclusions inside (i.e., when the microdroplet solution is undersaturated); and, (2) when there are solid inclusions inside of the microparticle (i.e., when the microdroplet solution is supersaturated). These two models will be developed for the particular case where energy dissipation of the microdroplet motion in the levitator atmosphere is linear.

Task Significance:

Understanding the metastable state evolution in supersaturated solutions is of extreme importance in the problem of governed nucleation and crystal growth. Since this evolution consists of the birth-death process of subcritical solute clusters, we outline the following significance:

1. It is a challenging experimental problem to study metastability since any heterogeneity may cause instantaneous nucleation followed by crystallization. Therefore, development of the containerless (without heterogeneities due to container walls) experimental technique is of interest.
2. Analytical description of stochastic motion of the confined supersaturated solution microdroplet will allow treatment of the obtained experimental data.

Progress During FY 1996:

1. Nucleation is a leading mechanism for many industrial processes such as sedimentation, purification, etc. One of the most difficult things to determine in connection with nucleation and prenucleation is the diffusivity of the subcritical solute clusters (embryos). For the first time we have found a theoretical description which connects diffusivity and viscosity with water activity above the microdroplet containing supersaturated water solution.
2. In the process of working with our experiments we have found that nucleation very often occurs before we reach the spinodal even in containerless microdroplets. The problem has been identified as having to do with impurities.

Because of this we have begun to assemble a device which will enable us to detect impurities down to a single molecule, and locate whether these impurities are in the bulk or on the surface of the droplet. The device is called an "Aerosol Particle Microscope (APM)." It owes its high resolution to a theoretical effort to understand the stochastic motion of a microparticle in an electrodynamic trap. This effort has led to a new principle for imaging Brownian particles in such a device, "Squeezed Imaging." A surprising result predicted by theory and confirmed by experiment is that Brownian motion of the particle's center of mass may be eliminated from long term images using a technique, which we termed "Squeezed Imaging." For surface molecules polarization selective imaging in inelastic scattering provides the orientation of the molecule relative to the surface normal. Further studies will connect the location and concentration of impurities with nucleation.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/94 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-25-08-30

NASA CONTRACT NO.: NAG8-975

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Arnold, S., Holler, S., Li, J.H., Serpengzel, A., Auffermann, W.F., and Hill, S.C. Aerosol Particle Microphotography and Glare Spot Absorption Spectroscopy. *Opt. Lett.*, 20, 773-775 (1995).

Arnold, S., Li, J.H., Holler, S., Korn, A., and Izmailov, A.F. Recording Long-Term Optical Images of a Brownian Particle in a Paul Trap essentially free of Thermally Induced Positional Noise. *J. Appl. Phys.*, 76, 1 (1995).

Izmailov, A.F., and Myerson, A.S. Concentration Dependence of Solution Shear Viscosity and Solute Mass Diffusivity in Crystal Growth from Solutions. *Phys. Rev. E*, 52, 805 (1995).

Izmailov, A.F., Arnold, S., Holler, S., and Myerson, A.S. Microparticle driven by Parametric and Random Forces: Theory and Experiment. *Phys. Rev. E*, 52, 1325 (1995).

Izmailov, A.F., Myerson, A.S., and Na, H.S. Supersaturated Electrolyte Solutions: Theory and Experiment. *Phys. Rev. E*, 52, 4 (1995).

Proceedings

Myerson, A.S., and Izmailov, A.F. "Study of Organic Supersaturated Solution: Theory and Experiment." *Crystal Growth of Organic Materials*, ACS, Washington, D.C., p 222 (1996).

Presentations

Izmailov, A.F., Myerson, A.S., and Na, H.S. "Supersaturated Electrolyte Solutions: Theory and Experiment." *American Institute of Chemical Engineers (AIChE) Annual Meeting*, Miami, Florida (1995).

Myerson, A.S., and Izmailov, A.F. "Thermodynamic Properties of Supersaturated Electrolyte Solutions." *The 13th Symposium on Industrial Crystallization*, Toulouse, France (1996).

Myerson, A.S., and Izmailov, A.F. "Fluctuation-Dissipation Theorem for Supersaturated Electrolyte Solutions." *The Tenth American Conference on Crystal Growth*, Vail, Colorado (1996).

Molecularly Tailored Surfaces via Self-Assembly Processes: Synthesis, Characterization and Modeling

PRINCIPAL INVESTIGATOR: Dr. Mark A. Barteau

University of Delaware

CO-INVESTIGATORS:

Lenhoff, A.M.

University of Delaware

Wagner, N.J.

University of Delaware

Task Objective:

The objectives of the proposed research are to develop experimental and theoretical techniques to design, fabricate, and characterize materials with specialized interfacial properties and to assess the role of gravitational forces in the fabrication of these materials. These materials will be synthesized by self-assembly of nanometer-scale and larger functional units. These units include polyoxometalates, proteins, lattices and polymers incorporating electronic, biological, and catalytic functions.

Task Description:

1. Preparation and characterization of ordered arrays. We use scanning tunneling microscopy (STM) to show that subunits as different in nature as inorganic oxide clusters and proteins spontaneously self-assemble into ordered arrays on graphite. We are exploring the generality of self-ordering phenomena by studying self-assembly of an expanded set of complex functions, including polyoxometalates, proteins and rod-like polymers, on a wider variety of surfaces using a more versatile set of techniques, in particular, atomic force microscopy (AFM).
2. Theoretical studies of array formation. More complete insight into self-ordering phenomena, particularly the capability to control the ordering for materials synthesis purposes, will be provided by theoretical studies to complement the experimental work. The theoretical component will comprise statistical mechanical analyses coupled with Brownian dynamics and Monte Carlo simulations. This will both facilitate the design of better experiments and have applicability in examining related problems in wetting and electrode performance, as well as provide important insights into adsorbate dynamics in the adsorbed layers.

Task Significance:

This research will develop experimental and theoretical techniques to design, fabricate, and characterize materials with specialized interfacial properties and assess the role of gravitational forces in the fabrication of these materials. The desired interfacial properties, to be derived from nanometer-scale and larger functional units self-assembled into ordered arrays at the interfaces of bulk materials, include electronic, biological, and catalytic functions. These include polyoxometalates as precursors to electronic and catalytic materials, proteins as precursors to biological materials such as affinity sorbents, biosensors, and other devices incorporating aspects of molecular recognition, as well as colloidal lattices and liquid crystalline polymers that have applications in corrosion-resistant coatings, tribology and membranes. The characteristic sizes of the adsorbates to be probed in this work span more than three orders of magnitude, from the nanometer to the micron scale, comparison and modeling of which will shed important light upon the underlying mechanisms of adsorption-induced self organization, and particularly the role of gravitational forces.

Progress During FY 1996:

1. Silicon Graphics workstation purchased and installed for theoretical studies of array formation.
2. Self-assembled monolayer formation demonstrated for four new polyoxometalates with anisotropic bulk structures.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/96 EXPIRATION: 7/00

PROJECT IDENTIFICATION: 962-21-10

NASA CONTRACT NO.: NAG8-124

RESPONSIBLE CENTER: MSFC

Studies of Nucleation and Growth of Intermetallic Compounds

PRINCIPAL INVESTIGATOR: Dr. Robert J. Bayuzick

Vanderbilt University

CO-INVESTIGATORS:

Hofmeister, W.H.

Vanderbilt University

Task Objective:

The objective of this research is to quantitatively define the nucleation behavior of selected intermetallic compounds and the relationship between the degree of undercooling and the speed of growth of the solid.

Task Description:

This work focuses on the undercooling of intermetallic compounds and their pure metal constituents by containerless processing. This ground-based research involves a continuation of already established drop tube work and electromagnetic levitation (on the bench). Specifics to be addressed are maximum undercoolings, nucleation frequency, the effect of undercooling on solidification velocity in refractory metals and alloys, and microstructural development as a function of deep undercooling/solidification velocity.

Research Approach

This work will consist of a comprehensive investigation on nucleation and growth of the solid from the undercooled liquid of selected intermetallics and their pure metal constituents. In order to do this, containerless processing is essential not only to eliminate the effect of the container on nucleation but also because the metals and alloys of interest are highly reactive and become contaminated with crucible material.

Three ground-based techniques for containerless processing will be applied to the effort. These are free fall in the long drop tube at the Marshall Space Flight Center, electromagnetic levitation "on the bench" at Vanderbilt University, and electrostatic levitation "on the bench" at the Jet Propulsion Laboratory.

The intermetallic compounds chosen to be studied initially are TiAl and NiAl. In addition, studies will be done on pure Ti and pure Ni, as points of reference and because of their standalone contribution to science. The particular intermetallics are chosen because both exhibit a wide solubility range as seen in their respective phase diagrams and, within composition ranges, exhibit a tendency to be unencumbered by competition between alternate phase selection in the deep undercooling regime.

Nucleation frequencies as a function of temperature will be obtained for each combination of specimen type and ground-based processing technique. In each case, the nucleation probability distribution and the cumulative distribution will be constructed from the nucleation frequencies. To do this, a large number of undercooling experiments on each specimen type will be conducted by each of the ground-based containerless methods. From analysis of the cumulative distributions, the kinetics of nucleation of the solid from the liquid for each specimen type under each processing condition will be quantitatively defined and examined in comparison to nucleation theory.

The ordered intermetallic alloys as well as their pure constituents will also be studied in order to determine the solidification velocity as a function of melt undercooling. The velocity will be determined using ultra high speed imaging to track the solidification front as it moves through the specimen. In opaque samples this can be done by monitoring the movement of the thermal field developed by recalescence. An instrument has been developed that consists of a 10 by 10 array of parallel tapped photodiodes and data acquisition. The system is capable of capturing data at rates of up to 1 million frames per second and the output from the array is calibrated for conversion to temperature. For each alloy and pure element, a plot of the solidification velocity as a function of undercooling will be developed. This data will be compared to present solidification theories and any areas of discrepancy will be addressed. Of particular interest are the mechanisms controlling the rate of solidification at various undercoolings.

Task Significance:

Intermetallic compounds and their composites are of considerable interest because of their potential use in high temperature structural applications. One strong driver for this interest is future goals for aircraft propulsion systems. Future aircraft engines will require high thrust-to-weight ratios and low specific fuel consumption, while remaining reliable, affordable, and highly maintainable. Effort involving innovative designs, advanced materials and processing, and improved design and analysis tools is required to meet Integrated High Performance Turbine Engine Technology goals for doubling propulsion system capabilities by the year 2005. Benefits of the required increase in engine cycle temperature must not be offset by increased turbine weight or cooling air. Thus, new materials and design technologies are needed for advanced high-temperature turbines.

The materials of interest in this study show potential for use in such applications because of their significantly increased high temperature strength and acceptable low temperature damage tolerance. It is therefore necessary to fully understand the nucleation and solidification behavior of these intermetallic compounds.

Progress During FY 1996:

The solidification velocity of Ti, γ -TiAl, γ -TiAl with dilute erbium additions, and equiatomic NiAl alloys has been measured. The results of these studies have been summarized by fitting the results with power laws.

The solidification velocity of pure titanium processed in ultra high purity helium (UHP He) was measured as a benchmark for the γ -TiAl study. The data indicated a continually increasing solidification velocity with increasing undercooling and was fit with the power law $V=0.057\Delta T^{2.5}$. This relation indicates a similar dependence of the solidification velocity of titanium as the dependence shown by pure nickel. However the difference between the materials is that the titanium data is fit by this power law over the entire undercooling range tested, while pure nickel indicated a discontinuity in the solidification velocity at $10\%T_M$ undercooling.

The γ -TiAl solidification velocity data showed three solidification regimes. They were: 1) for $\Delta T < 9\% T_M$ the velocity increased slowly with increasing undercooling, 2) for $9\% T_M < \Delta T < 18\% T_M$ the velocity increased rapidly with increasing undercooling, and 3) for $\Delta T > 18\% T_M$ the functional dependence of the solidification velocity on the undercooling was greatly reduced with the velocity remaining around 10 m sec^{-1} up to 20% undercooling.

The power law fits for the three solidification regimes shown by γ -TiAl are presented in Table 1 along with the power law fit for pure Ti processed in UHP He.

Table 1 - Summary of the power law fits for the γ -TiAl alloy.

Material	Power Law	Undercooling Range
Ti in UHP He	$V=0.057\Delta T^{2.5}$	$8\% T_M < \Delta T < 14.4\% T_M$
γ -TiAl	$V=0.17\Delta T^{0.89}$	$\Delta T < 9\% T_M$
γ -TiAl	$V=0.014\Delta T^{2.25}$	$9\% T_M < \Delta T < 18\% T_M$
γ -TiAl	$V \approx 10 \text{ m/s}$	$\Delta T > 18\% T_M$

The effect of dilute additions of the substitutional element erbium on the solidification behavior of γ -TiAl was also measured. The 0.25 and 0.5 a/o erbium addition alloys show increasing velocities with increasing undercooling up to $\Delta T \approx 10\% T_M$, above which point they remain constant at about 4 m/s. The 1 a/o erbium alloys have very slow solidification velocities at all undercoolings. The results indicate that the velocity increases with increasing undercooling up to the maximum achieved undercooling, $16\%T_M$. At this maximum undercooling the velocity is about 1 m/s.

Solidification theory for ordered intermetallic alloys predicts a transition from solidification of the ordered phase to solidification of a disordered phase with increasing solidification velocity and increasing undercooling. Boettinger and Aziz (Acta Metall., V.37, p.3379, 1989) estimated the critical velocity above which ordered phase solidification could not take place for γ -TiAl as 0.6 m/s. The results of this study indicate the transition from solidification of ordered TiAl to solidification of disordered TiAl at approximately 1.4 m/s corresponding to $9\%T_M$ undercooling. The transition is evident in the data set by the increased dependence of the solidification velocity on undercooling

after this solidification velocity was reached. Solidification of disordered TiAl in this regime was also indicated by the direct observation of the subsequent ordering reaction of the disordered phase. Additionally, microstructural indications of primary solidification of the disordered phase were observed in a companion study. (Kral, Bassler, Hofmeister, and Wittig, Mat. Res. Soc. Symp. Proc., V.364, p.1995)

Undercoolings of 11% T_M and 13.1% T_M were obtained for equiatomic NiAl processed in UHP He. Corresponding solidification velocities were 1.9 m/s and 2.5 m/s.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 9/94 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 962-25-08-20

NASA CONTRACT NO.: NAG8-108

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Bassler, B.T., Hofmeister, W.H., and Bayuzick, R.J. "Examination of Solidification Velocity Determination in Bulk Undercooled Nickel." MRS Fall Meeting, Boston, Massachusetts, December 1995.

Hofmeister, W.H., Bassler, B.T., and Bayuzick, R.J. "Measurement of High Speed Solidification Events." International Symposia on Advanced Materials and Technology for the 21st Century, The 117th Meeting of JIM, Honolulu, Hawaii, December 1995.

Transport Phenomena During Equiaxed Solidification of Alloys

PRINCIPAL INVESTIGATOR: Prof. Christoph Beckermann

University of Iowa

CO-INVESTIGATORS:

de Groh III, H.C.

NASA Lewis Research Center (LeRC)

Task Objective:

To investigate the macrosegregation and structural inhomogeneities resulting from gravity-induced thermosolutal convection and solid sedimentation during equiaxed solidification of alloys on a bulk level.

Task Description:

The melt flow and solid transport phenomena occurring during equiaxed alloy solidification are investigated in experiments using both metal alloys and transparent analogues. The drag and heat/mass transfer coefficients of single equiaxed crystals are measured by employing fabricated dendrite models and, *in situ* using transparent model alloys. This information is combined to develop a multi-phase/-scale simulation model that allows for the calculation of the individual solid and liquid motions during solidification and incorporates the detailed phase interactions on a microscopic scale.

Task Significance:

This investigation complements NASA-sponsored research on the influence of fluid flow in alloy casting by including the important effects of gravity-induced motion of free equiaxed crystals. This combined experimental and theoretical/numerical study will provide (1) needed fundamental understanding of how liquid convection and the movement of free equiaxed grains interrelate and produce segregation and structural zones in castings, (2) progress towards a more complete numerical simulation model of transport and solidification phenomena, and (3) a base for defining future microgravity flight experiments on equiaxed dendritic solidification.

Progress During FY 1996:

Bulk solidification experiments using Al-Cu alloys have been performed. An analysis of the compositional and structural patterns achieved in the experiments is presently underway. This data is intended for comparison with predictions from the numerical simulation model.

Considerable progress has been made in measuring the mass transfer coefficient of single growing equiaxed transparent model alloy crystals settling in an undercooled melt. Additional experiments were conducted using a succinonitrile-acetone alloy. Simultaneous measurements of the dendrite tip growth velocities are also being analyzed.

A multi-scale/-phase model of equiaxed dendritic alloy solidification with melt convection and transport of free crystals has been developed. Detailed comparisons of the model predictions with the Al-Cu alloy experiments (see above) are being carried out.

The findings of this research have also been used to develop future microgravity experiments involving the growth and interactions of multiple equiaxed dendrites, known as Equiaxed Dendritic Solidification Experiment (EDSE).

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	2	MS Degrees:	1
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 11/93 EXPIRATION: 1/96

PROJECT IDENTIFICATION: 962-25-05-23

NASA CONTRACT NO.: NCC3-290

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Song, H., Tewari, S.N., and de Groh III, H.C., Convection during thermally unstable solidification of Pb-Sn in a magnetic field. *Met. and Mat. Trans. A*, vol. 27A, pp. 1095-1110. (April 1996).

Wang, C.Y. and Beckermann, C., Equiaxed dendritic solidification with convection: Part 1, multi-scale/-phase modeling. *Met. and Mat. Trans.*, (1996).

Wang, C.Y. and Beckermann, C., Equiaxed dendritic solidification with convection: Part 2, numerical simulations for an Al-4wt%Cu alloy. *Met. and Mat. Trans.*, (1996).

Wang, C.Y. and Beckermann, C., Equiaxed dendritic solidification with convection: Part 3, comparisons with NH₄Cl-H₂O experiments. *Met. and Mat. Trans.*, (1996).

Presentations

Beckermann, C. and Wang, C.Y., "Modeling of microstructure formation in alloy solidification with convection." JIM Annual Meeting, 1996.

Equiaxed Dendritic Solidification Experiment

PRINCIPAL INVESTIGATOR: Prof. Christoph Beckermann

University of Iowa

CO-INVESTIGATORS:de Groh III, H.C.
Steinbach, I.NASA Lewis Research Center (LeRC)
Access e.v. (Germany)

Task Objective:

To study the microstructural evolution of and thermal interactions between several equiaxed crystals growing dendritically in an undercooled melt of a pure substance.

Task Description:

1. To perform experiments using the transparent model material SCN and a modified version of the Millikelvin Thermostat (MITH), where up to four equiaxed crystals are grown towards each other. Also, to measure the orientation and shape of the crystals, the temporal variation of the velocities of the primary and secondary dendrite tips, dendrite arm spacing and thicknesses, and melt temperatures at selected locations as a function of the initial undercooling.
2. To perform corresponding ground-based experiments and measurements; visualize and measure the flow field in the growth chamber; explore the possibilities of varying the crystal spacings and measuring the volume change due to phase change (to determine the fraction solidified); compare to microgravity data and quantify the influence of convection.
3. To perform mesoscopic simulations of selected experiments in the limit of diffusional heat transport, using the measured crystal orientations and dendrite tip velocities, as well as initial and boundary conditions, as input; perform inverse analyses to back out the thermal undercoolings responsible for the observed tip velocities as well as to calculate the solid fraction evolution behind the tips; if possible, compare the latter to the experiments; explore the possibility of performing mesoscopic numerical simulations including thermal convection in order to better model the ground-based experiments.
4. To deduce a refined unit-cell (or volume averaged) model of equiaxed dendritic solidification from the mesoscopic simulations for the diffusion case and, ultimately, extend it to the case with convection.
5. To perform microscopic phase field simulations to further the understanding of the underlying physical mechanisms associated with the growth of isolated and multiple dendrites.

Task Significance:

In recent years the widened availability of powerful computers and commercial casting simulation software has bridged the once wide division between basic solidification research and foundry practice. Computer simulation is used in the foundry industry to design defect-free castings and improve quality. The simulations are generally based on heat and fluid flow analyses at the scale of the casting and provide the temperature distribution, cooling rates, and solidification progress during casting. A major recent development in this area has been the coupling of such simulations with models of microstructural evolution during solidification. The microstructure plays a key role in determining the mechanical properties of a material. Thus, the use of coupled casting/microstructure simulations allows for the selection of process conditions that optimize the properties of a material for a given processing technique. Despite the significant progress made in recent years, many microstructural evolution models are based on highly simplified physical scenarios and have never actually been experimentally verified completely. The proposed microgravity experiment is designed to provide much needed benchmark data for the testing and refinement of microstructure growth models, for use in coupled micro-/macroscopic casting simulations.

Nearly all solidification in metal alloy castings occurs in a dendritic mode. Dendrites are classified as being either constrained or free. The former grow from a surface in a columnar fashion and are only found in materials that freeze

over a temperature range and when growth takes place into a positive temperature gradient. Such directional solidification has been the subject of numerous studies and a number of theories have been proposed to predict the undercooling, velocity, and radius of curvature of the dendrite/cell tip and, also, the primary spacing of a dendrite array. Constrained growth will not be considered further. Free dendrites are those which are "nucleated" and grow in an equiaxed fashion in supercooled liquid and can occur in both pure materials and materials exhibiting a freezing range. Several aspects of equiaxed solidification are well enough understood to model accurately. The growth of an assemblage of free equiaxed crystals and a concomitant understanding of equiaxed growth are the subjects of the proposed research.

Progress During FY 1996:

The kick off meeting was held at LeRC with the Professor Beckermann (PI) and the engineering team on June 19, 1996. The PI gave an overview of his experiment and requested a chamber to grow crystals. The team will design and build a growth chamber and isothermal bath for the PI capable of growing up to four crystals simultaneously. The most recent concept is to have four dendrites originate from each corner of a tetrahedron since this is an efficient space filling arrangement. This geometry would be placed inside of a cube; the cube becomes the external shape of the growth chamber. Tests will be conducted at the University of Iowa.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 9/96 EXPIRATION: 9/99

PROJECT IDENTIFICATION:

NASA CONTRACT NO.: NCC8-94

RESPONSIBLE CENTER: LeRC

Gravitational Effects on the Development of Weld-Pool and Solidification Microstructures in Metal Alloy Single Crystals

PRINCIPAL INVESTIGATOR: Dr. Lynn A. Boatner

Oak Ridge National Laboratory

CO-INVESTIGATORS:

David, S.
Workman, G.Oak Ridge National Laboratory
University of Alabama, Huntsville (UAH)

Task Objective:

The objectives of this research are to achieve an in-depth quantitative understanding of the role played by natural, convection-driven, and surface-tension-driven heat and mass transport in determining the shape and surface morphology of fusion melt pools and, thereby, to control the nature of the solidification processes that determine the microstructural and mechanical properties of welds and castings.

Task Description:

By combining ground-based results with those obtained in the low- and high-g environments provided by NASA aircraft, detailed microstructural information can be obtained through the use of single-crystal alloy specimens, and both gravitational and surface-tension-driven effects on weld-pool formation and microstructural properties can be delineated and quantified. The results of these investigations are currently yielding new information that is serving to advance our level of understanding of various phenomena which determine both weld-pool shapes, mass transport, and the morphological properties of solidification surfaces.

This research represents a new and innovative approach to the investigation of gravitational effects on melt-pool shapes, solidification phenomena, surface morphology, and weld microstructures. This approach is based on the application of our recently developed alloy single-crystal methods for the delineation of solidification microstructural properties and on the new quantitative analytical methods that have been developed in conjunction with the unique experimental results that can be obtained through the application of these single-crystal techniques. This approach to the study of weld and solidification microstructures begins with the growth of macroscopic single crystals of the alloy system that is to be investigated. As in the case of our previous studies, oriented Czochralski-grown single crystals of the pure ternary alloy 70Fe-15Ni-15Cr (a compositional analog of one of the 300 series of stainless steels) are being utilized. Palladium is deposited on the single-crystal samples to serve as a tracer element in mapping mass transport phenomena.

Task Significance:

The long-term goal of this research effort is to achieve a firm scientific basis for the development of a comprehensive scientific program in which more-complex solidification and welding experiments can be carried out on NASA aircraft, on Space Shuttle flights, and eventually on the International Space Station. Since the microstructural properties of weld pools and the distribution of certain impurities within the weld are central to determining the weld mechanical strength, these experiments have practical implications regarding a wide range of construction, fabrication, and manufacturing operations both in space and on earth.

Progress During FY 1996:

The diversity of forces that result in mass transport phenomena and free-surface-deformation effects in melt pools coupled with the individual complex nature of these interactions makes the development of comprehensive solidification models extremely difficult. Accordingly, experimental data are needed that represent the results of controlled experiments on simplified model systems and configurations. Experiments have been carried out in which oriented, high-purity single crystals of a ternary alloy (an analog of a 300 series stainless steel) were used to achieve dramatic simplifications in the solidification microstructures formed in stationary melt pools. Additionally, the low-gravity environment provided by the NASA DC-9 aircraft has been used to minimize the effects of gravitational forces on mass transport and, accordingly, on the melt-pool shape and associated solidification microstructure.

Several large single crystals of a stainless steel alloy whose composition is 70%Fe-15%Ni-15%Cr (all in wt. %)

were grown by means of the Czochralski technique in preparation for the series of experiments that was subsequently performed in August 1996 on the NASA DC-9 aircraft flying out of the NASA Lewis Research Center. These single-crystal boules were oriented using Laue x-ray back-reflection techniques, and oriented slices were then cut from the boules using electric-discharge machining (EDM) in order to minimize the introduction of damage into the single-crystal samples.

Three types of specimens were prepared for the DC-9 investigations. One set of samples consisted of uniform circular disks that were EDM machined to a diameter of 0.9", lapped to a thickness of 0.09", and then polished with colloidal silica. Thirty-six of these samples were used in DC-9 experiments designed to investigate the influence of low and high-g (≈ 2 g) conditions on stationary melt-pool shapes and solidification-cell properties. The second sample type consisted of a "sandwich" configuration in which two single-crystal disks were plated on one side of each disk with a 0.005"-thick coating of palladium. The Pd-coated faces were then placed in contact while preserving a common in-plane crystallographic orientation for the two single-crystal halves. This configuration was then stabilized with small laser welds made on the periphery of the crystals. Six of these "sandwich" specimens were used on the DC-9 flight in experiments based on our recently developed technique of tracer mapping of fluid flow in metal melts. In this approach, a stationary melt pool is initially formed using (in the case of the DC-9 experiments) a gas-tungsten-arc heat source. When the penetration depth of the melt pool reaches the palladium layer, molten palladium is introduced and is then transported according to the existing liquid-flow patterns. The melt pool is then allowed to solidify and the palladium distribution is subsequently mapped in cross-section samples by means of scanning electron microscopy/secondary electron emission techniques.

The third sample type utilized in the DC-9 flight experiments consisted of single ternary alloy crystal disks that were plated with palladium on the top surface except for a small circular area located in the center of the sample. Six of these specimens were used in investigations in which the Pd tracer was introduced into the surface (as opposed to introduction at the bottom of the pool as in the case of the "sandwich" specimens) of the melt pool - but only after the melt-pool diameter had increased to the point exceeding that of the circular area that was not plated with palladium.

Metallographic cross sections have been prepared, etched, and examined for the 36 unplated single crystal disk samples flown on the DC-9 aircraft. The microstructural properties of the solidified melts, including determinations of the dendritic solidification-cell diameters under low- and high-g conditions, are currently being analyzed. Similar analyses are in progress for the palladium-plated "sandwich" and top-surface Pd-coated specimens.

The morphological properties of the surface formed by the solidification of stationary single-crystal melt pools was investigated in considerable detail resulting in a new level of understanding of capillary-wave dynamics and how periodic collective motions of the molten liquid leads to the formation of frozen-in "ripples" on the solidified surface. These ripples are in the form of concentric bands whose frequency increases as the diameter of the liquid phase decreases during solidification. The amplitudes and effective wavelengths of the capillary-wave-produced oscillatory surface features are currently being analyzed in the case of the single crystal samples flown on the DC-9 aircraft. In the course of the investigations of surface ripples formed by capillary wave motion, new global surface morphological effects, whose magnitude is up to two orders of magnitude larger than the surface ripples, have been found. These effects are currently under investigation since they clearly can affect mass transport in solidifying melt pools.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	1
MS Students:	2	MS Degrees:	1
PhD Students:	1	PhD Degrees:	0

TASK INITIATION: 2/93 EXPIRATION: 2/96

PROJECT IDENTIFICATION: 962-25-08-23

NASA CONTRACT NO.: H-13059D

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Boatner, L.A., Corrigan, D., David, S.A., Rappaz, M., Workman, G., and Smith, G. "Surface Morphological Properties of Stationary Melt Pools in Single Crystals of Stainless Steel." NASA Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Dispersion Microstructure and Rheology in Ceramics Processing

PRINCIPAL INVESTIGATOR: Dr. John F. Brady

California Institute of Technology (Caltech)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Better ceramic materials and parts may be obtained through careful control of the processing of ceramic suspensions. Monodisperse particle suspensions have met with limited success even though the maximum volume fraction that can be achieved prior to sintering is 0.74. This may stem from the fact that a perfect crystal of mono-sized particles has slip planes that yield easily, and from the fact that there is still a large amount of void space that must be eliminated upon sintering. An alternate approach is to use a mixture of particle sizes. Solids fractions of 90% can be obtained with a bidisperse suspension of spherical particles, and slip planes can be eliminated. In addition, a mixture of two different types of particles can also impart desirable properties in a 'composite' ceramic. The objective of this research is to understand the behavior of bidisperse suspensions under flow so that improved processing of ceramics is possible.

Task Description:

Microstructure formation and rheology of concentrated bidisperse suspensions will be investigated by a combination of Stokesian Dynamics simulation and analytical modeling. Unbounded shear flows and slip-casting will be simulated, and the influence of particle size ratio, volume concentration, shear rate and thermal energy on microstructure formation determined. Analytical models will be developed to predict structure formation and flow behavior during ceramics processing. Owing to size or compositional differences, particle mixtures are subject to gravitational phase separation or demixing, and microgravity processing may provide an attractive environment for producing advanced ceramics.

Task Significance:

Ceramics provide a potentially very useful class of materials owing to their physical properties: they are light, hard, resistant to abrasion, chemically inert, stable at high temperatures, and excellent thermal and electrical insulators. Further, by casting from a liquid suspension and subsequently sintering (baking), many complex parts and shapes can be fabricated. High-performance ceramics produced from monodisperse particulate suspensions have not fulfilled their promise owing to defects produced during sintering. Improved ceramic materials may be obtained by using a mixture, either by size or composition, of fine particles. Critical to the success of such a mixture is the control of the dispersion microstructure during processing, which is the focus of this research.

Progress During FY 1996:

Funding for this project started recently on April 22, 1996; progress has, therefore, been modest. We are currently implementing a strategy to render the Stokesian Dynamics simulation method more efficient, specifically reducing the computational burden from an $O(N^3)$ to an $O(N)$ algorithm, where N is the number of degrees of freedom. This task will occupy the bulk of 1996-1997. It is necessary in order to simulate the behavior of bidisperse colloidal dispersions, which may be used in ceramics processing.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 4/96 EXPIRATION: 4/97

PROJECT IDENTIFICATION: 962-21-26

NASA CONTRACT NO.: NAG8-123

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Brady, J.F. "Dispersion Microstructure and Rheology in Ceramics Processing (poster exhibit)." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Combustion Synthesis of Materials in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Kenneth Brezinsky

University of Illinois, Chicago

CO-INVESTIGATORS:

Law, C.K.
Glassman, I.Princeton University
Princeton University

Task Objective:

Homogeneous suspensions of metal particles in supercritical nitrogen that can only be formed in a microgravity environment are proposed as the subject of this new study. Microgravity is a crucial part of the experimental program because of three unique effects of this type of environment on the proposed experiments. The first and key effect is that particle settling can be inhibited so that a true homogeneous suspension critical to a novel synthesis approach can be obtained. Specifically, a nitride synthesis approach has been proposed in which the nitride product would be generated from a flame propagating through a controlled density suspension of titanium particles in nitrogen at temperatures and pressures just past the critical point (supercritical nitrogen). This approach offers advantages both as a process technique and as a means of scientific study, namely: 1) The suspension provides a more porous medium than a solid powder compact or a loose bed for transport of nitrogen to reacting particles; 2) The high (approximately 40 atmospheres) but not extremely high pressure provides an adequate and more convenient supply of nitrogen, without bubble formation, for the complete reaction of individual titanium particles; 3) The density and therefore concentration of nitrogen for the limit of kinetically controlled product formation is controllable because of the almost infinite isothermal compressibility near the critical point; 4) The particles can be sufficiently separated by varying and maintaining at microgravity the particle density of the suspension so that, in principle, agglomeration is not a problem; 5) The burning intensity can be controlled by varying and maintaining at microgravity the particle suspension density; and, 6) The final titanium nitride product will be in the form of powders whose shapes and sizes are in principle controllable through the selection of the initial titanium particles and, at microgravity, unaltered by settling. Such shape and size specific powders are expected to be of great commercial value.

The second effect is that a microgravity environment eliminates the hydrostatic pressure that exists on Earth in a column of fluid simply due to its weight. This hydrostatic pressure varies with position in a vertical column of fluid. For properties of supercritical fluids which are extremely sensitive to pressure, as is the density near the critical point, variations will exist, on Earth, along the column length. To avoid these variations and maintain a homogeneous supercritical nitrogen environment, a microgravity based experimental program is paramount.

A third advantage of microgravity conditions is to provide a "containerless" environment. The quartz and stainless steel materials that will contain the titanium powder have been shown to contribute to the contamination and reduced yield of the nitride product. In microgravity, suspensions can be created and maintained so that wall effects are minimized.

Task Description:

Initial experiments will be aimed at the design and development of a means of formation of a uniform suspension of powder particles in supercritical nitrogen. Subsequent experiments in a microgravity environment will focus on obtaining spatially resolved temperature and particle characteristics across the flame. The microgravity environment envisioned for the initial research is that available on the DC-9 aircraft.

Task Significance:

Uniform suspensions of metal particles in supercritical nitrogen that can only be formed in a microgravity environment are proposed as the subject of this new study. Microgravity is a crucial part of the experimental program because of the unique effects of this type of environment on the proposed experiments. Specifically, a materials combustion synthesis approach has been proposed in which the nitride product would be generated from a flame propagating through a controlled density suspension of titanium particles in nitrogen at low temperatures and high pressures just past the critical point (supercritical nitrogen). The knowledge gained in this microgravity

experiment, because the particles won't settle out during the synthesis, will be essential for understanding the combustion synthesis of hard, high temperature and chemical resistant powders of controlled shape and size. Such shape and size specific powders are expected to be of great commercial value because, in principle, they can be processed to form objects with superior properties.

Progress During FY 1996:

This program began very late in FY96 and consequently progress during the fiscal year was limited. In the short duration of the program, two articles - one based on previous NASA supported research and the other an extensive review of related research, were prepared. The initial design for the formation of heterogeneous suspensions was also begun.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 **EXPIRATION:** 4/00

PROJECT IDENTIFICATION: 962-21-34

NASA CONTRACT NO.: NAG8-126

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Brezinsky, K. "Gas-Phase Combustion Synthesis of Materials." Twenty-Sixth Symp. (Int.) Comb., The Combustion Institute (1996).

Brezinsky, K., Brehm, J.A., Law, C.K., and Glassman, I. "Supercritical Combustion Synthesis of Titanium Nitride." Twenty-Sixth Symp. (Int.) Comb., The Combustion Institute (1996).

Presentations

Brezinsky, K., Brehm, J.A., Law, C.K., and Glassman, I. "Supercritical Combustion Synthesis of Titanium Nitride." 1996 Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.

Modeling of Convection and Crystal Growth in Directional Solidification of Semiconductor and Oxide Crystals

PRINCIPAL INVESTIGATOR: Dr. Robert A. Brown

Massachusetts Institute of Technology (MIT)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The research underway in this program focuses on the development of detailed models and simulation tools for analysis of the interactions of heat and solute transport on the quality of crystals grown from the melt by the vertical Bridgman (VB) method and in small-scale floating zones. The crystal growth of germanium and silicon in the FZ method and of an oxide (Bismuth Germanate) are under investigation.

Task Description:

The research is aimed at developing detailed simulations of both the vertical Bridgman (VB) and floating zone (FZ) methods and at using this simulation capability to answer important questions about the dynamics of these crystal growth methods as operated in both earth-bound and microgravity conditions. The research has been divided into several subtasks:

- Development of an integrated model for the vertical Bridgman crystal growth method;
- Development of an integrated model for analysis of small-scale floating zones;
- Development of finite element methods for analysis of these models;
- Extension of the methods to parallel computation and to three-dimensional modeling; and,
- Applications of these analyses to particular crystal growth systems.

The results of these studies are important because fundamental understanding of the interactions of heat, mass, and solute transport affect the quality of crystals grown from the melt. Moreover, the analysis will lead to interpretation of results from experiments and to algorithms for the design and control of systems for crystal growth. An integrated model has been developed of VB growth for this purpose. The analysis combines heat transfer throughout the furnace by radiation between all elements, conduction in all phases, and convection in the melt, with calculation of the solidification interface. Convection in the melt is driven by buoyancy and phase change. Radiation in the crystal and melt are included in the analysis of analysis of oxide materials. All analysis assumes axial symmetry around the axis of the furnace and crystal. The model for a small-scale FZ includes heat transfer by conduction, convection in the melt, and radiation to and from the surroundings. The shapes of the melt/crystal interfaces and the meniscus are found as part of the analysis. Steady-state calculations are carried out using finite-element/Newton methods. Analysis for the VB system has focused on the development of iterative numerical methods for the solution of the very large, asymmetric linear equation sets that arise from the finite element discretization and Newton's method. Our approach to the solution of this problem is to use iterative methods with a high degree of parallelizability so that clusters of moderate-sized engineering workstations can be used for three-dimensional analysis.

Task Significance:

The techniques for analysis and the insights gained from the analyses supported by this program have broad application to a variety of ground-based and space flight experiments supported by NASA and its European and Japanese counterparts. Interactions between this modeling effort and NASA sponsored experimental programs have shown that modeling and carefully controlled ground-based experiments are crucial to performing well-controlled space experiments. The detailed simulation of vertical Bridgman (VB) growth and the modeling of floating zone systems has direct applicability for these systems.

Progress During FY 1996:

Significant progress has been made on two research fronts: the development of dynamic and stability analysis for small-scale floating zones and the development of numerical methods for parallel computation of convection in melt crystal growth.

The analysis of small-scale floating zones reported earlier has been extended to include a detailed analysis of floating zone stability to disturbances caused both perturbations of meniscus shape and to hydrodynamic instability for flows caused by thermocapillary forces, buoyancy or zone rotation. Our study is the first analysis of small-scale floating zones to be based on an integrated model of the hydrodynamics and zone shape. The approach is based on using the finite-element model for axisymmetric, steady-state heat transfer and melt convection, and analyzing the stability of these flows to three-dimensional, small amplitude perturbations to these states. The perturbations are represented by a combination of finite element approximation in the meridional plane and azimuthal Fourier decomposition. This approach leads to a very large set of linear, constant-coefficient differential algebraic equations or to a generalized eigenvalue problem with a high degree of singularity. We have developed two approaches for solving this problem. In the first, a preconditioned Arnoldi iterative method is used to compute the most dangerous eigenvalues. The algorithm combines recent advances in using backward difference methods for preconditioning of the Krylov iteration with estimates for convergence for the eigenvalues. The stability calculations have been applied to the analysis of experimental results for flow transition in model floating zones formed with silicon oils and molten salts. The calculations give quantitative description of the transitions in the stability from axisymmetric thermocapillary motion to three-dimensional steady and time-dependent flows in these experiments.

We have successfully developed a family of iterative methods based on the BICGSTAB version of Krylov iterations, coupled with domain decomposition based matrix preconditioner adapted from the additive and multiplicative Schwarz methods. Tests with a classical test problem from buoyancy-driven convection show that the Schwarz/Krylov methods are almost a factor of ten more efficient on a single processor machine than a very efficient domain decomposition implementation of direct factorization. Preliminary tests on parallel versions of the code show that the parallel efficiency is higher for the iterative method, as expected. The Schwarz/Krylov methods are now being implemented for solution of the entire linear equation set resulting from the integrated model of vertical Bridgman (VB) growth.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	3	PhD Degrees:	1

TASK INITIATION: 7/93 **EXPIRATION:** 12/96

PROJECT IDENTIFICATION: 962-21-08-17

NASA CONTRACT NO.: NAG8-961

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:
Journals

Covert, H. and Brown, R.A. Dynamics of small-scale floating zones: The thermal capillary limit. MIT Report, (1996).

Mehrabi, M.R. and Brown, R.A. Parallel implementation of finite-element/Newton method for solution of steady-state and transient nonlinear partial differential equations. J. Sci. Computing, 10, 93-137 (1995).

*Microstructure Formation During Directional Solidification of Binary Alloys Without Convection:
Experiment and Computation*

PRINCIPAL INVESTIGATOR: Dr. Robert A. Brown

Massachusetts Institute of Technology (MIT)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

A combination of experimental and theoretical research will be aimed at developing a predictive understanding of cellular and dendritic microstructures of dilute binary alloys and lamellar spacing in the growth of eutectics formed during thin-film solidification. The results will form the basis for prediction of the dependence of microstructure formation on macroscale properties of bulk solidification systems, such as the imposed temperature gradient and the sample growth rate.

Task Description:

The extensive theoretical and experimental research on microstructure formation point to the formation of cellular microstructures in binary alloys and lamellar eutectics as being formed under conditions of long time-scale, spatiotemporal chaos in the pattern. These patterns involve a band of wavelengths that evolve with changes in the operating conditions, such as growth rate and temperature gradient, and include very long wavelength interactions through which the pattern communicates over length scales much larger than the characteristic cell size. The outstanding problem that will be addressed in the research is to begin to construct mean field models for solidification microstructure that are based on microscopic mechanics of individual elements in the microstructure. Experimental, theoretical and computational studies will be conducted that will lead toward this goal. These elements of the research plan are:

- Experimental studies of spatiotemporal chaos in cellular solidification and the role of externally applied forcing functions on regularization of the pattern;
- Extension of the analysis of wavelength selection to thin-film eutectic solidification;
- Experimental studies of lamellar eutectic growth in thin-film solidification; and
- The development of stochastic and mean field models for pattern formation in directional solidification.

The microstructure of metal alloys formed from directional solidification plays an important role in the mechanical and electrical properties of these materials. This investigation describes experimental and theoretical research aimed at developing a predictive understanding of cellular and dendritic microstructures of dilute binary alloys and the lamellar spacing in the growth of eutectics formed during thin-film solidification. The combination of experimental and theoretical results will form the basis for prediction of the dependence of microstructure formation on macroscale properties of bulk solidification systems, such as the imposed temperature gradient and the sample growth rate. The experimental studies are carefully designed so that bulk convection, driven by density gradients, is unimportant. In this way, the results are applicable to gravity-free experiments that will be undertaken during space flight. The theoretical framework for understanding nonlinear pattern formation during solidification is so complex that there is little hope of unraveling the mechanisms for pattern formation in the presence of convection without rigorous analysis and experiment in the absence of convection. The thin-film experimental geometry offers the only mechanism for accomplishing this goal on Earth.

Task Significance:

The research has the promise of making significant progress towards the development of a theoretical framework for characterizing the formation of microstructure in alloy solidification. The experiments and microscale calculations to be conducted will lay the foundation for detailed description of the mechanisms for length scale adjustment in cellular and lamellar eutectic growth. The development of kinetic theory for describing the evolution of the microscale will give the connection between processing variables and microscale formation that is necessary for

adaptation of the theory to practice in industrially important systems, and will provide a framework for the characterization of alloy systems for microstructural modeling parameters.

Progress During FY 1996:

Analysis of the dynamics of cellular directional solidification requires numerical methods capable of dynamic simulation of large collections of cells for long times compared with the dynamics of individual cells. We have developed such a method based on the simulation of cellular solidification on a fixed Cartesian grid. Here finite difference approximations are used to describe solute transport and the melt/crystal interface is interpolated within the grid and advanced in time. The fixed grid method has been formulated with the two-sided solutal model used by us in previous simulations of cellular solidification. The method generalizes to models with simultaneously varying heat and solute transport.

The fixed grid method advances the melt/crystal interface semi-explicitly in time. For a given interface shape at an instant in time, the partial-differential equations describing solute transport are solved by a Crank-Nicholson, centered difference scheme using the Gibbs-Thomson equation to describe the solute concentration along the interface in terms of its curvature at the previous time step. The normal velocity of the interface is then computed from the interfacial solute balance. Given this distribution of normal velocity along the interface at the previous time step, the interface shape is advanced using a dynamical description of the geometry that leaves points along the interface equally distributed in arc-length. In this description, no assumptions are made about the representation of the melt/solid interface relative to any particular coordinate system so that deep and reentrant interface shapes can be computed. The accuracy of these shapes is only limited by the number of points along the interface and by the finite difference grid, which sets the accuracy of the concentration field and hence the calculation of the interface velocity.

The algorithm has been tested by computation of the morphological stability criterion for a planar interface in the limit of small amplitude perturbations. The agreement with the linear stability theory is excellent. Calculations for single cells and small clusters of cells have been compared with results of our group and are in good agreement, showing transitions for steady state growth to time-periodic and chaotic dynamics among the cells. Calculations for very large collections of cells are planned during the remainder of this grant.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	0
PhD Students:	0	PhD Degrees:	1

TASK INITIATION: 7/93 EXPIRATION: 12/96

PROJECT IDENTIFICATION: 962-25-08-25

NASA CONTRACT No.: NAG8-962

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Kyrilidis, A. and Brown, R.A. Density functional theory of melt-solid interfaces in hard sphere systems. *Physical Review E*, 51, 5832-5845 (1995).

Xia, Y. and Brown, R.A. Measurement of the onset of two-dimensional cellular solidification in the succinonitrile-acetone binary alloy. *J. Crystal Growth*, 154, 205-210 (1995).

Application of Parallel Computing for Two- and Three-Dimensional Modeling of Bulk Crystal Growth and Microstructure Formation

PRINCIPAL INVESTIGATOR: Dr. Robert A. Brown

Massachusetts Institute of Technology (MIT)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The quality of metal, oxide, and semiconductor crystals grown from the melt depends fundamentally on heat, mass, and species transport in the melt and crystal and on the interactions of these fields with the formation of microdefects, dislocations, and voids in the grown crystal. The research program described here focuses on the development of simulation tools for analysis of detailed, integrated models of melt crystal growth systems. To be quantitative for modeling microgravity experiments such models must be three-dimensional and, many times, time dependent, and must include convection in the melt, heat transfer by conduction, radiation, and convection in all phases, and species transport in the melt phase. Most importantly, the models must couple together these transport processes to yield an integrated picture of transport throughout the system. The proposed research intends to develop finite-element based analysis of such models, coupled with numerical algorithms for the solution of these models that are particularly adapted for use of scalable parallel computing. These software tools will make the analysis accessible to a wide range of engineers and scientists working on crystal growth problems.

Task Description:

The first goals of this research are to develop robust algorithms for the solution of integrated models of melt crystal growth to allow the analysis of such systems. An important feature of this proposal is the application of scalable parallel computing, where scalable parallel computers can be either clusters of workstations connected by a low-performance network, such as an ethernet, or aggregates of such workstations that are self-contained in one unit and connected by a high-performance fiber optic link. The numerical algorithms are being built around the finite-element/Newton methods that we have developed with good success for the solution of material processing models that represent complex physico-chemical hydrodynamics and transport. These algorithms combine accurate finite element discretizations of the field equations and boundary conditions, quasi-orthogonal mapping methods for coupling the action of free- and moving-boundaries, local mesh refinement for capturing features of these solution fields, and Newton's method for solution of the nonlinear algebraic equations that arise in the solution of steady-state problems or in implicit integration methods for transient problems. Efficient implementation on parallel computers requires algorithms for the solution of the linear algebraic equations that arise at each Newton iteration. We are pursuing this approach using two methods: (i) a concurrent factorization and storage algorithm (CFS) for direct solution of asymmetric, indefinite, linear algebraic equations, and (ii) Schwarz/Krylov methods for preconditioned iterative solution of these equations.

Task Significance:

Modeling of individual transport processes and understanding their complex interactions in crystal growth systems is fundamentally important to the successful growth of crystals in a microgravity environment and to the interpretation of experiments from ground-based and microgravity research. The research described here will aid these goals by supplying simulation methods, as well as results for particular systems for these applications.

Progress During FY 1996:

This program was initiated very late in the funding year; hence, the number of results that have been specifically funded by this contract are small. The initial research has focused on a direct comparison of parallel versions of direct and iterative methods for solution of a prototype, two-dimensional natural convection problem discretized with classical finite element methods. The linear equation solvers are used to solve the equations arising at each iteration of Newton's method. The two methods are the concurrent factorization and storage algorithm (CFS) developed by us under a previous contract and a Krylov-based iterative method using additive and multiplicative Schwarz preconditioners. Both methods use domain decomposition methods and are implemented on parallel computers using this approach. The CFS method is a Schur decomposition method; the resulting Schur complement matrix also is factorized directly in parallel.

Calculations for two-dimensional natural convection in a cavity show that the CFS method is 4-6 times more efficient than conventional LU decomposition software based on frontal factorization methods. Computation times on a single processor of an IBM SP2 computer show an additional factor of six speed improvement for the Krylov/Schwarz method over the CFS algorithm. The speed increase is expected to be larger for the parallel implementation because the Krylov/Schwarz should have a substantially higher parallel efficiency than the 65% that is typical for the CFS algorithm.

We are developing a three-dimensional version of this software to test the robustness of the algorithms and the scalability of the results for calculation of three-dimensional buoyancy-driven flow in a cavity. This is the first step toward the development of fully functional three-dimensional simulations of convection in crystal growth systems such as the vertical Bridgman system used in several flight experiments.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/96 EXPIRATION: 5/99

PROJECT IDENTIFICATION: 962-21-03

NASA CONTRACT No.: NAG8-125

RESPONSIBLE CENTER: MSFC

Evolution of Crystal and Amorphous Phase Structure During Processing of Thermoplastic Polymers

PRINCIPAL INVESTIGATOR: Prof. Peggy Cebe

Tufts University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Our objective is to study microstructure evolution during melt processing and secondary thermal treatment of high performance thermoplastic polymers which are candidate materials for advanced composite applications. We will investigate formation of structure in both the crystalline and the amorphous phases. The purpose of the study is to determine the effects of processing conditions on the resultant structure and physical properties of thermoplastics. We hope to address the manner in which self-deformation stresses affect the microstructure of the solidifying polymer melt. Processing in a microgravity environment will impose very different stress states on molten polymers during solidification, compared to ground-based processing conditions. Dependence of polymer microstructure and physical properties on processing conditions can more easily be predicted and controlled under microgravity conditions where self-deformation forces are avoided.

Task Description:

Present ground-based processing methodologies requires gravity compensation to support the processed piece during solidification. Therefore nearly all melt processing approaches (e.g., extrusion, film blowing, fiber drawing) involve very rapid quenching of the molten material to avoid imposing self deformation stresses on the melt. Rapid quenching results in inhomogeneous cross-sections, since the center of the piece cools more slowly than the exterior. In a microgravity environment, it would be possible to use very slow melt processing techniques to obtain more uniform microstructure throughout the section, minimizing the morphology gradient between the skin and the core of the section.

The proposed research is a ground-based study of slow melt processing in the gravity environment. We will process thermoplastic polymers by solidification from the melt without gravity compensation. First we will use real-time x-ray scattering at elevated temperature to study the kinetics of solidification. Then we will examine the resultant microstructure at room temperature after processing. Self deformation stresses on the melt will be studied to determine the effects of gravity on the development of crystalline structure and morphology from the (stressed) amorphous melt. We will characterize the unit cell structure of the crystal phase, the disposition of unit cells within the crystals, and the organization of crystals into larger units such as spherulites, fibrillar bundles, or shish-kebab structures. We will also study the amorphous phase structure to determine degree of chain alignment and the amount of rigid vs. mobile amorphous phase. Additionally, the location of rigid vs. mobile amorphous chains with respect to the crystals will be examined.

The principal approaches used in this study will be real-time wide and small angle x-ray scattering, which will be performed at the Brookhaven National Synchrotron Light Source and in our in-house x-ray laboratory. In addition, we will use differential scanning calorimetry, optical microscopy and birefringence to characterize the polymers after processing. Standard mechanical tests, such as stress-strain and impact resistance measurements, will be used to study the performance of the test pieces. One unique aspect of the proposed research is the combined study of both the crystal and the amorphous phases. We will be concerned not only with the nucleation and growth of crystals, but also with residual stresses and chain alignment in the amorphous phase.

Task Significance:

Our ultimate goal is to contribute to a fundamental understanding of microstructure evolution in thermoplastic polymers solidifying under influence of self deformation stresses, and to determine the ameliorating effects of the microgravity environment. Once we know the effect of self deformation stress during processing, we will be better able to predict the solidification behavior of polymers in the microgravity environment. This will lead to development of unique processing applications that capitalize on the microgravity environment. Complementary experimentation under reduced gravity conditions would later be proposed to be performed on the Space Shuttle or

on Space Station. Ground-based facilities, such as drop towers and KC-135, would not provide the capability for real-time studies of microstructure development under practical processing conditions.

Progress During FY 1996:

As part of our study of amorphous and crystalline orientation in polymers, real-time high temperature small angle X-ray scattering experiments were conducted at the Brookhaven National Synchrotron Light Source. A small injection molding device was constructed and tested. We successfully injected polyethylene melt into the mold cavity at high temperature, and monitored the x-ray pattern in real time. As the melt crystallizes, it forms oriented crystallites which use the preoriented melt as the template for crystal growth. In complementary studies performed in-house, the optical birefringence of the preoriented melt was monitored using laser optical ellipsometry. This provides an immediate indication of preorientation in the melt, before any long range crystalline order has been established.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 3
MS Students: 0
PhD Students: 1

TASK INITIATION: 12/94 EXPIRATION: 12/96

PROJECT IDENTIFICATION: 962-26-08-12

NASA CONTRACT No.: NAG8-111

RESPONSIBLE CENTER: MSFC

Optical Properties for High Temperature Materials Research

PRINCIPAL INVESTIGATOR: Dr. Ared Cezairliyan

National Institute of Standards and Technology

CO-INVESTIGATORS:

Krishnan, S.

Containerless Research, Inc.

McClure, J.

National Institute of Standards and Technology (NIST)

Task Objective:

The objective of this research is to obtain definitive values for the normal spectral emissivity of selected high-melting-point metals by two independent techniques in order to provide a foundation for reliable radiometric temperature measurements in materials research at high temperatures, both in microgravity and on the ground.

Task Description:

The research will include accurate measurements of the normal spectral emissivity of selected metals near and at their melting points in a series of subsecond pulse-heating experiments in which the emissivity will be determined at two laser wavelengths in the range 0.5-0.9 μm by two independent techniques involving high-speed pyrometry and laser polarimetry, respectively. The simultaneous measurements by the two techniques on the same specimen will minimize a number of major experimental uncertainties, in particular those arising from specimen surface conditions and specimen purity.

Task Significance:

The results of this research will enable the establishment of reference values for normal spectral emissivity (also leading to high temperature radiometric standards) which are critically needed for accurate temperature measurements in materials research on high-temperature liquids and melts and in the determination of their thermophysical properties at high temperatures, under either microgravity or terrestrial conditions. In addition, the proposed work will resolve the current major controversy in the scientific literature regarding the wavelength dependence of normal spectral emissivity of metals at and near their melting points.

Progress During FY 1996:

As the results of extensive tests performed in our laboratory, the high-speed laser polarimeter was modified to improve stability of the optical system, calibration procedure, and ease of overall operation related to optical alignment and data processing. Experiments were conducted where normal spectral emissivity of tungsten was measured in the temperature range 2000 to 3500 K. The results obtained by the new laser polarimetric technique and the conventional radiometric method were in an excellent agreement (within 1%). Definitive measurements related to the application of the laser polarimetric technique to the non-contact detection of phase transformation were performed. The measurements included detection of structural phase transformations (titanium, zirconium, iron, and hafnium) and melting (nickel, zirconium, 53Nb-47Ti alloy, and a commercial nickel-base alloy). As an additional test of the operation of the laser polarimeter, the specific heat capacity of molybdenum was measured in the temperature range 2000 to 2500 K, where true temperature was determined based on the normal spectral emissivity obtained from the laser polarimetric measurements. The agreement of the results with the established values of the specific heat capacity values of molybdenum (standard reference material) is within 1%.

This three-year project was successfully completed during FY96. Based on the extensive tests conducted and the results obtained on several materials, it can be concluded that the high-speed laser polarimetry is a reliable technique for measuring normal spectral emissivity of materials in millisecond-resolution pulse-heating experiments at high temperatures.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 3/93 EXPIRATION: 3/96

PROJECT IDENTIFICATION: 962-25-08-27

NASA CONTRACT No.: H-18067D

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Cezairliyan, A., and Righini, F. Issues in High-Speed Pyrometry. Metrologia, vol. 33, 299-306 (1996).

Kaschnitz, E., and Cezairliyan, A. Radiance Temperatures at 1500 nm of Niobium and Molybdenum at Their Melting Points by a Pulse-Heating Technique. Int. J. Thermophys., vol. 17, 1069-1078 (1996).

Presentations

Cezairliyan, A. "Thermophysical Properties of High Temperature Liquid Metals and Alloys." NASA Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.

Kaschnitz, E., McClure, J., and Cezairliyan, A. "Radiance Temperatures (in the Wavelength Range 500-1500 nm) of Cobalt and Iron at Their Melting Points by a Pulse-Heating Technique." 14th European Conference on Thermophysical Properties, Lyon, France, September 1996.

Thermophysical Properties of High Temperature Liquid Metals and Alloys

PRINCIPAL INVESTIGATOR: Dr. Ared Cezairliyan

National Institute of Standards and Technology

CO-INVESTIGATORS:

Krishnan, S.

Containerless Research, Inc.

Task Objective:

The objective of this research is to extend, for the first time, the laser polarimetry technique for measuring normal spectral emissivity to the microsecond time regime. This will enable accurate determination of the true temperature of liquid specimens at high temperatures in rapid pulse heating experiments. In addition to the measurement of other experimental quantities, the proposed project will yield data on selected thermophysical properties with unsurpassed accuracy that can be used in support of microgravity related research. The properties to be measured include enthalpy, specific heat capacity, heat of fusion, and electrical resistivity above the melting temperatures of selected high-melting-point metals and alloys.

Task Description:

An ultra-fast laser polarimeter will be developed for use in microsecond-resolution pulse-heating experiments to enable measurements of normal spectral emissivity (at 650 nm), which in conjunction with the measurement of radiance temperature, will yield the true temperature of liquid materials. The system will be used to accurately measure selected thermophysical properties (enthalpy, specific heat capacity, heat of fusion, and electrical resistivity) of selected high-melting-point liquid metals and alloys at temperatures above 1500 K and up to about 4000 K. Additionally, studies will be made to establish the nature of thermodynamic equilibrium in these fast experiments vis-a-vis steady-state techniques, like levitation melting.

Task Significance:

Thermophysical property values for liquid metals and alloys are needed in modeling solidification and crystal growth, in containerless processing, and for casting and welding design. A number of these processing techniques are currently being practiced in the reduced gravity environment. Our research supports these efforts by providing reliable thermophysical measurements methodology and accurate thermophysical properties data on selected key materials.

Progress During FY 1996:

This task began in May 1996. Feasibility of developing an ultra-fast laser polarimeter for the accurate measurement of normal spectral emissivity in microsecond-resolution experiments was studied. A breadboard device was constructed to simulate some of the critical operations of the laser polarimeter under extreme conditions of high heating rates at high temperatures. This device was tested in microsecond-resolution (1-10 MHz rate) pulse-heating experiments on molybdenum. The specific purposes of the tests were to (a) assess the performance of the polarimeter electronics under actual experimental conditions, (b) assess the performance of the optical system, and (c) assess and identify important experimental parameters. Design of the self-contained microsecond-resolution laser polarimeter has begun. It is anticipated that the construction of the prototype laser polarimeter will be completed by the end of FY97.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-21-35

NASA CONTRACT NO.: H-23799D

RESPONSIBLE CENTER: MSFC

Three-Dimensional Velocity Field Characterization in a Bridgman Apparatus: Technique Development and Effect Analysis

PRINCIPAL INVESTIGATOR: Dr. Soyoung S. Cha

University of Illinois, Chicago

CO-INVESTIGATORS:

Betha, M.D.

NASA Lewis Research Center (LeRC)

Task Objective:

The objective of the proposed research is to provide means for measuring three-dimensional (3-D) three-component (3-C) velocity fields and characterizing important solidification parameters in crystal growth. In this effort, two unique complementary diagnostic techniques will be developed, closer to a state appropriate for microgravity experiments (i.e., holographic diffraction image velocimetry (HDIV) and stereo-imaging velocimetry (SIV)). The simultaneous development of HDIV and SIV is desirable because of their complementary nature with respective strengths and limitations. These two techniques together can cover a broad range of space experiment requirements including complex or transient phenomena. The developed techniques are then employed to observe the flow fields in a typical crystal growth configuration. In addition to the velocity measurements, other pertinent information will also be extracted from the experiments and then these will be compared with those from numerical modeling.

Task Description:

HDIV, utilizing high-quality high-resolution holographic imaging, can provide good spatial resolution, accuracy, and dynamic range with experimental freedom in field observation and measurement of hard-to-reach regions. However, it does not allow real-time monitoring. It is also immature in development and disadvantageous in system complexity. One task is to bring the technique to a practical level through efficient software/hardware development and system miniaturization. SIV is relatively mature and advantageous in system simplicity and real-time monitoring. However, it has weaknesses in limited detection capability, utilizing low-resolution solid-state imaging. These two approaches thus exhibit contrasting characteristics. Another task is to further improve the SIV system for efficient experimental monitoring. The last task is to set up experiments for verifying the proposed approaches and extracting various useful information.

Task Significance:

The structural perfection of crystal growth strongly depends on the influence of thermally-induced flows in the liquid phase, which act in a detrimental manner. In both ground-based and space-based processing, these velocity fields need to be measured to identify their effects on the processing. In spite of the efforts to stabilize fluid flow problems, their influence cannot be completely eliminated. Consequently, measurement of three-dimensional (3-D) three-component (3-C) velocity fields is very essential for optimizing production parameters. The experimental velocity characterization is also vital to validation and improvement of numerical process modeling. The proposed Bridgman configuration is one of the most basic arrangements and its investigation is of great technological importance. The ultimate goal of this proposal is to expand the application to space-based experiments in the future through technique perfection and hardware miniaturization, not only for crystal growth but also for other allied areas.

Progress During FY 1996:

In the previous five months since the start of this new project, a substantial effort has been directed toward the preparation of the future research activities. These involve organizing general strategies, which can include examination of the theoretical investigation approaches, formation of the initial structures in software development, and initial design of the hardware setups.

For theoretical fundamental investigation, a study for characterizing the design effects of various miniaturized optical components is initiated in preparation of the miniaturization of the holographic-diffraction-image-velocimetry (HDIV) system and its application to material processing experiments. As an example, the image distortion can be caused by change in reconstruction laser wavelength, shrinkage of plastic roll film, etc. All these effects are under investigation to minimize the experimental errors through calibration.

HDIV employs cross-correlation and cross-product operations for three-dimensional velocity information extraction. Efficient computational algorithms, which are based on the fast Fourier transform, are being investigated for integration into the system. The study of interpolation schemes for achieving the accuracy substantially below the sampling interval is also under way.

Design of two new hardware systems for HDIV and stereo-imaging-velocimetry (SIV) is in progress to build miniaturized prototype instruments. These involve examination of component specifications, design parameter calculations, and compatibility and performance estimation. The preparation of an initial experiment for HDIV is also under way with a breadboard-type instrument before building a prototype system for checking the performances of all the sub-techniques which have been developed to date.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 4/96 EXPIRATION: 4/97

PROJECT IDENTIFICATION: 962-21-11

NASA CONTRACT NO.: NAG8-124

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Slepicka, J.S., and Cha, S.S. "Holographic Diffraction Image Velocimetry for the Measurement of Three-Dimensional Velocity Fields." AIAA-96-2265, presented at the 19th AIAA Advanced Measurement and Ground Testing Technology Conference, New Orleans, Louisiana, June 1996.

Microgravity Chemical Vapor Deposition

PRINCIPAL INVESTIGATOR: Dr. Ivan O. Clark

NASA Langley Research Center (LaRC)

CO-INVESTIGATORS:

Jesser, W.A.

University of Virginia

Hyer, P.V.

Lockheed Martin

Johnson, E.J.

Lockheed Martin

Task Objective:

This research will develop a better understanding of the scientific principles underlying chemical vapor deposition (CVD). The proposed research will determine to what extent microgravity can elucidate and separate these competing phenomena and will form the basis for a proposal to perform a series of flight experiments to more fully elucidate these scientific principles.

Task Description:

Ground-based experimental and numerical investigations will provide both basic scientific information on the heat and mass transfer effects central to the CVD process and define specific follow-on reduced-gravity investigations. This multi-pronged approach will maximize the utilization of available resources and capabilities. In the numerical modeling, both finite difference and spectral element techniques will be used and the predictions compared. In the experimental phases of the effort, a horizontal CVD reactor design will be used for the growth of a model material, such as aluminum, and a commercially important material, InP. Laser velocimetry measurements of the flow fields in the reactor will also be performed.

Task Significance:

CVD is an extremely important industrial technique with applications in the fields of semiconductors, optics, and corrosion resistance. The nature and quality of the layers formed are dependent on mass and energy transport as well as homogeneous and heterogeneous chemical reactions and nucleation. Commercial CVD processes currently employ reactors developed through decades of empirical trial and error. Scientific understanding of the CVD process is limited by the difficulty of separating the heat and mass transport due to externally forced convection and that of the internal processes of buoyant thermal convection, buoyant solutal convection, and thermal (Soret) and solutal diffusion. There is also forced convection due to volume changes arising from both reactive chemistry and thermal effects. A better understanding of these effects is essential to achieve desired improvements in perfection, uniformity, and size of grown layers and to provide an engineering design basis for these systems.

Progress During FY 1996:

Thermal imaging and particle imaging velocimetry (PIV) techniques have been applied to a model chemical vapor deposition (CVD) reactor. The thermal imaging provided much improved boundary conditions for use in the numerical modeling effort. It also demonstrated that jets were present in the reactor when hydrogen test gas was used and that the thermal image of these jets could be used as a diagnostic tool to improve the repeatability of experiments in CVD reactors. These results strongly suggest that applying thermal imaging to industrial process plants could result in improved factory yield. Technology transfer efforts to investigate this application are being developed.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 11/92 EXPIRATION: 11/95

PROJECT IDENTIFICATION: 962-21-06-09

RESPONSIBLE CENTER: LaRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Clark, I.O., Hyer, P.V., and Johnson, E.J. "Thermal imaging for enhanced semiconductor process yield." Technology 2006, Anaheim, CA, October 29-31, 1996.

Clark, I.O., Jesser, W.A., Hyer, P.V. and Johnson, E.J. "Microgravity chemical vapor deposition." Microgravity Materials Science Conference, Huntsville, AL, June 10-11, 1996.

Glass Formation and Nucleation in Microgravity: Containerless-Processed, Inviscid Silicate/Oxide Melts (Ground-Based Studies)

PRINCIPAL INVESTIGATOR: Dr. Reid F. Cooper

University of Wisconsin, Madison

CO-INVESTIGATORS:

Perepezko, J.H.

University of Wisconsin, Madison

Task Objective:

1. Nucleation by internal oxidation or reduction of transition metal-bearing silicate glasses and melts.

If a change in valence state of a transition metal cation within a silicate melt is associated with a change in its structural role within the melt, one might be able to effect internal homogeneous nucleation within the melt via a change in the external environment, for example, by a redox reaction. Critical to the hypothesis is the nature of transition metal cations to make the melt into a semiconductor: Conduction electrons or electron holes are majority defect species and thus serve to decouple cation and anion diffusion fluxes that occur in an oxygen chemical potential gradient. One consequence is that oxidation or reduction reactions can occur internally (i.e., within the body of the melt) instead of solely on the surface. These reactions can result in the destabilization of the melt such that crystallization reactions occur in finely (nm-scale) dispersed regions of the melt body (e.g., the formation of Fe^{3+} -bearing spinel precipitates via the internal oxidation of an originally Fe^{2+} -bearing aluminosilicate melt). One can thus create fine-grained glass-ceramics from what would normally be non-glass-forming melts. Specific research involves control reaction experiments on silicate glasses and levitated reaction experiments (aero-acoustic and electrostatic levitation) on silicate melts.

2. Internal nucleation of inviscid pseudobinary silicate melts via metastable liquid-phase immiscibility.

Binary alkaline Earth oxide-silicate melts are highly exothermic. Nevertheless, the structural variations between highly polymerized (silica-rich) and poorly polymerized (silica-poor) silicate liquids result in the creation of composition zones (on the silica-rich end of the phase diagram) where a single silicate liquid is not stable. On the silica-poor end of the diagram, this immiscibility would be metastable. As a consequence, if one can sufficiently undercool an inviscid, silica-poor melt, one could perhaps cause metastable amorphous-phase separation to occur prior to any crystallization. The phase separation could further promote the internal, fine (μm)-scale, uniform nucleation and crystallization of the material. The creation of unique glass-ceramic materials becomes a possibility. Scientifically, measurements of heat evolution rate in such droplets will address questions concerning the role of amorphous phase separation in crystalline nucleation.

Task Description:

Two research approaches are employed for the two tasks:

1. Containerless processing for oxidation of Fe^{2+} -bearing alkaline Earth aluminosilicate melts via aero-acoustic levitation (AAL). Small droplets (~3mm diameter) of ferrous iron-bearing calcium aluminosilicate glass, prepared initially by bulk melting in a controlled-oxygen activity furnace, are levitated and remelted using AAL and laser heating. The droplets thus formed are evaluated for their surface reactions, using Rutherford backscattering spectroscopy (RBS), and for their internal reactions using analytical transmission electron microscopy (AEM and TEM). The kinetics of the redox reaction are evaluated as functions of temperature, time, and oxygen activity, the latter controlled via the gas used as a levitation medium. The results of these experiments are compared to those done at low temperature on glasses of identical composition; with such a check, the study can be later extended to melts too inviscid to be glass formers. The nature of nucleation as affected by local oxygen fugacity will be explored using electron diffraction study of the internal oxidation front.

2. Drop-tube processing of pseudobinary silicate melts. Binary MgO-SiO_2 metasilicate compositions near the deep cristobalite (SiO_2)-enstatite (MgSiO_3) eutectic are melted in a drop tube. Initially fine, crystalline powder, the fine droplets are allowed by the degree of undercooling to experience metastable phase separation. Those droplets receiving sufficient undercooling to additionally penetrate the glass transition can be thermodynamically analyzed to explore the nature of nucleation in phase-separated amorphous materials. Primary analysis tools of the processing

include secondary electron emission microscopy (scanning electron microscope), X-ray diffraction, TEM and electron microdiffraction, and differential thermal analysis and scanning calorimetry. These data should allow discrimination of the role of amorphous-amorphous interfaces on crystalline nucleation in the phase-separated amorphous droplets. The study will be extended to the binary $\text{Al}_2\text{O}_3\text{-SiO}_2$ system, the alumina-rich end producing highly inviscid melts that, if sufficiently undercooled, could produce interesting alumina/mullite glass-ceramics.

Task Significance:

Both of the specific tasks in this research are critically dependent on containerless processing: in both cases, avoiding containers eliminates the most blatant source of heterogeneity's that could promote heterogeneous nucleation. In the case of redox reactions (Task 1) the containerless requirement is additionally (and particularly) important in that chemical (as opposed to structural, e.g., nucleation reactions can grossly affect the ionic-scale dynamics and structure of a transition metal-bearing melt. For example, noble-metal crucibles (e.g. platinum) that are often employed to contain refractory ionic melts will alloy with the transition metal ions incorporated in the melt: chemical diffusion different from that desired in the redox experimental results.

Microgravity comes into play when working with inviscid ceramic melts, specifically in the same two manners cited for dealing with molten metals : (1) density contrast amongst phases and (2) the need for quiescence. Both of these aspects are evident in our levitated melt drop experiments: melt viscosities of approximately 1 Pa.s (10 Poises) allow for shear-force-induced convection (droplets are far too small for thermal convection at this viscosity; processing of modestly larger melt bodies could promote thermal convection), which allows continuous exposure of new melt to the outside atmosphere thus short-circuiting the desired chemical diffusion process; in droplets avoiding convection, Ostwald ripening of internally formed ferrites allows them to sink to the bottom of the droplet, thus removing them from positions to act as internal nuclei for silicate phases.

Progress During FY 1996:

Structural and dynamical models for redox reactions in vitreous and molten iron-bearing aluminosilicate melts were developed and applied to the experimental data collected earlier in the task. We have characterized clearly the applicability of percolation models for the modifier cations in vitreous/amorphous aluminosilicates. We demonstrate that internal oxidation and reduction reactions are sufficiently rapid that one can establish criteria for "isothermal undercooling" through the propagation of an oxidation or reduction front through a liquid. Reduction experiments show capability of application of ideas to transition metal cation-doped inviscid oxide melts: microgravity processing would be critical to the success of the approach.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	2
PhD Students:	1	PhD Degrees:	0

TASK INITIATION: 12/91 EXPIRATION: 1/96

PROJECT IDENTIFICATION: 963-26-07-01

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Cooper, R.F., Fanselow, J.B. and Poker, D.B. The mechanism of oxidation of a basaltic glass: Chemical diffusion of network-modifying cations. *Geochim Cosmochim. Acta*, 60, 3253-3265 (1996).

Cooper, R.F., Fanselow, J. B., Weber, J.K.R., Merkley, D.R. and Poker, D.B. Dynamics of oxidation of a Fe^{2+} -bearing aluminosilicate (basaltic) melt. *Science*, 274 (1996).

Proceedings

Cooper, R.F. "Dynamic redox reactions and the formation of fine-grained, polycrystalline oxide/silicate ceramics from inviscid melts." In: *Space Processing of Materials*, edited by N. Ramachandran, Proc. SPIE, 2809:69-77 (1996).

Fundamental Studies of Solidification in Microgravity using Real-Time X-Ray Microscopy

PRINCIPAL INVESTIGATOR: Dr. Peter A. Curreri

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Kaukler, W.F.

University of Alabama at Huntsville (UAH-CMMR)

Sen, S.

Universities Space Research Association (USRA)

Bhat, B.N.

NASA Marshall Space Flight Center (MSFC)

Task Objective:

The objective is to utilize X-ray Transmission Microscopy (XTM) to provide direct measure of the solute profile in the liquid, phase coalescence and growth in the liquid, and the detailed interface morphology (e.g., dendrites and cells) during solidification of metal alloys and semiconductors in microgravity.

Task Description:

This research will obtain fundamental measurements of the dynamics of solidification in metallic or semiconducting materials with microstructural resolution. These data will be used to test the classical type boundary layer theories as applied to microgravity solidification. The data will also be applied to test coupled growth theories to the microgravity solidification of eutectics and monotectic alloys.

Task Significance:

This research applies a state of the art sub-micron source to image (with resolutions up to 25 micrometers) the solidification of metallic or semiconductor alloys in real-time. We have successfully imaged in real-time: interfacial morphologies, nucleation, coalescence, incorporation of phases into the growing interface, and the solute boundary layer in the liquid at the solid-liquid interface. We have also measured true local growth rates and can evaluate segregation structures in the solid. The ability to image these features in real-time will enable more fundamental and detailed understanding of solidification dynamics in microgravity than had previously been possible, thus allowing the full benefits of microgravity experiments to be applied towards rigorous testing of critical solidification models.

Progress During FY 1996:

Al-1.5 w/o Pb monotectic alloys were unidirectionally solidified. X-ray transmission microscopic (XTM) observations, both during and after solidification, revealed various new morphological/compositional features in the melt and solid. In the melt, nonuniform lead-rich interfacial segregation layers and droplets were observed. In the solid, periodic striae formed at translation/solidification velocities down to 6 $\mu\text{m}/\text{sec}$. Their shape does not replicate that of the interface. Their spacings, which decrease with increasing solidification rate, range from 200 - 400 microns for rates between 16 and 6 microns/s. Post-solidification XTM examination at higher resolution reveals that these striae consist of Pb-rich particles of 2-3 microns diameter. At translation/solidification velocities below 6 microns/sec, Pb incorporation into the solid occurs in the form of continuous fibers and strings of particles of about 5 micron diameter. Bands, parallel to the interface, in which these fibers were aligned in the solidification direction, alternated with bands of poor fiber alignment. The width of these bands is comparable to the striae spacings obtained at the high solidification rates.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-21-04

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Curreri, P.A., and Kaukler, W. Real-Time X-Ray Transmission Microscopy of Solidifying Al-In Alloys. Metallurgical Transactions, vol. 27A, no. 3, 801-808 (1996).

Sen, S., Dhindaw, B.K., Stefanescu, D.M., and Curreri, P.A. Melt Convection Effects on the Critical Velocity of Particle Engulfment. J. of Crystal Growth, (August 1996, accepted).

Proceedings

Curreri, P.A., and Kaukler, W. "X-Ray Transmission Microscopy Study of the Dynamics of Solid/Liquid Interfacial Breakdown During Metal Alloy Solidification." Proceedings of the 8th International Symposium on Experimental Methods for Microgravity Materials Science, 125 TMS Annual Meeting, Anaheim, California, February 4-8, 1996.

Kaukler, W.K., and Curreri, P.A. "X-Ray Transmission Microscopy of Al-Pb Monotectic Alloys During Directional Solidification." Proceedings of the 8th International Symposium on Experimental Methods for Microgravity Materials Science, 125 TMS Annual Meeting, Anaheim, California, February 4-8, 1996.

Kaukler, W.K., and Curreri, P.A. "Advancement of X-ray Microscopy Technology and its Application to Metal Solidification Studies." Proceedings of the 1996 SPIE Technical Conference in Space Processing of Materials, paper #5, pp 34-44, Proceedings Vol. 2809, N. Ramachandran, ed., August 4, 1996.

Sen, S., Dhindaw, B.K., Stefanescu, D.M., and Curreri, P.A. "Melt Convection Effects on the Critical Velocity of Engulfment in the Biphenyl/Glass Particles system." Proceedings of the 8th International Symposium on Experimental Methods for Microgravity Materials Science, 125 TMS Annual Meeting, Anaheim, California, February 4-8, 1996.

Directional Solidification in ^3He - ^4He Alloys

PRINCIPAL INVESTIGATOR: Prof. Arnold Dahm

Case Western Reserve University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The goal of this research is to enhance our fundamental understanding of crystal growth kinetics, liquid-solid interface morphologies, and the stability of alloys.

Task Description:

Preliminary observations of dendritic growth in two-dimensional samples of ^4He and mixtures growth of the planar interface have been made. Systematic studies of cellular and dendritic growth in ^3He - ^4He alloys will be conducted to complement work that has been done in other alloys. Attempts to observe the initial instability of the planar interface will by undertaken.

Task Significance:

The study of morphologies is of intrinsic interest in testing theories of non-linear systems. Results which differ from those of classical alloys will guide both theorists and experiments in their future studies, and significant differences should result in new ideas for space-based alloy growth experiments. ^3He - ^4He alloys have a large advantage over other alloys in that the parameters which control the interface morphology, such as the latent heat, thermal conduction, ^3He mean free path, and the phase diagram (temperature versus concentration), can be varied over a large range by a small change in temperature or solute concentration.

Progress During FY 1996:

The goal of this research is to observe dendritic and cellular growth of the in ^3He - ^4He alloy interface in regions with different values of the parameters which control the interface morphology and, in particular, in the temperature range near 1.4 K where the melting curves for different concentrations of ^3He cross.

In our experiment solidification is driven by a pressure differential at constant temperature. Solidification occurs at pressures ≥ 25 atm. Our initial attempts to observe cellular patterns led to some unforeseen difficulties. These include difficulty with consistency in sealing of glass windows onto the cell, ^3He convection currents in our cell, blocking of the fill capillary with the solid phase, growth of the solid phase on the inner sides of our bellows which supply the alloy to the cell, and lack of control of location of the interface in our cell.

The difficulty in sealing windows was resolved with a new technique of epoxying indium shims between the glass windows and brass frames of our cell. Convection problems were greatly reduced and possibly eliminated by placing a sieve in front of the inlet (fill) capillary through which helium is added to increase the pressure to a value greater than the melting pressure to supercool the sample. The rest of the problems were associated with wetting of metals with the solid phase of our alloy.

Pure solid helium does not wet metals. However, we discovered that with arbitrarily small concentrations of ^3He the solid phase would begin to grow from the metallic sides of the cell instead of advancing from the horizontal solid-liquid interface in the cell. In addition, the fill capillary would block when solid wet the walls of the capillary. We undertook a study of wetting by the solid phase of ^3He - ^4He alloys on different materials. We found that preferential wetting of the solid phase of alloys occurs in order of decreasing wetting on brass, epoxy, stainless steel, and indium, and the solid phase does not wet glass. We have solved the problem of fill capillary blockage and growth on bellows by replacing our CuNi capillary with stainless steel fill lines and replacing our copper bellows with stainless steel bellows. We have designed our sieve which prevents convection currents by drilling small holes in a piece of brass shim stock and coating all parts of the sieve including the channels with indium. Our present cell has glass front and rear portions for viewing and a brass frame on the sides. The brass sides of the cell are coated with indium, the top is covered with our indium coated sieve, and the bottom from which the solid phase

is grown is brass. We are presently fabricating a similar cell with thin glass replacing the indium coating the sides of the cell. Each step of improvement has increased our ability to control the location of the interface. Our last attempt to study dendrites and cellular growth indicated some difficulty with growth of the solid phase on epoxy which was squeezed into the cell during fabrication. This problem should be easily resolvable.

Our preliminary investigations have been in two directions: attempts to study the onset of instability of the planar interface, and dendritic and cellular morphologies of the interface. After initial attempts, we worked to eliminate problems such as convection currents and undesired locations of wetting of surfaces by the solid before proceeding to a more extensive study. Our work to date has been with a 100 ppm ^3He concentration. Before some of our recent improvements, we were able to grow a planar hcp solid interface at arbitrarily small velocities. However, at some particular interface velocity dendritic growth suddenly appeared on a brass surface near the top of the cell so that the initial instability of the planar interface could not be studied. We believe that this was due to convection ^3He currents and having brass surfaces in contact with the sample. We were unable to grow a planar interface of the bcc solid phase of the alloy. We do not know whether this is an inherent problem or a difference in wetting properties of the hcp and bcc phases.

It is straight forward to observed dendritic growth of the interface at larger interface velocities. We made preliminary measurements on two-dimensional samples of the alloy and pure ^4He . Dendritic tips under some conditions, those which we studied, are of dimensions of 1 - 3 mm, while our cell thickness is 0.5 mm. Thus, heat flow is restricted to a plane. The boundary conditions on equations describing two-dimensional dendritic growth differ from the three-dimensional case. Some of the patterns we observed appeared to be cellular, although we are not sure of this. We believe that we have resolved the most severe problems which have interfered with a controlled study, and will begin a systematic study when our glass coated cell is sealed.

Our program is to first study the instability of the planar interface at different temperatures (different parameters). We will study the differences in planar growth of the hcp and bcc interfaces. Then dendritic growth and cellular growth will be studied. We expect to have initial phases of these investigations at a 100 ppm concentration to be finished by October 1, 1995. Further studies will include a more extensive study of the above and a study at different solute concentrations which will probe different parts of the phase diagram.

We have studied the interface morphology as a function of interface velocity for a ^3He - ^4He alloy with a concentration of 500 ppm ^3He . Planar, cellular and dendritic morphologies were observed. This effort is being carried out by a undergraduate student. Much of the effort was directed toward changes in cell design to reduce convection currents of the solute. Presently, we are attempting to study the statistical variations of the changes in morphologies. Our goal is to grow a large number of crystals at different interface velocities near the transition from planar to cellular growth and from cellular to dendritic growth. The probability of cellular (dendritic) growth [the fraction of times cellular (dendritic) growth occurs within a fixed time will be plotted versus interface velocity with a goal of understanding the resultant statistics.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 0

TASK INITIATION: 1/92 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-25-05-25

NASA CONTRACT NO.: NAG3-141

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Chen, M.T. and Dahm, A.J., Optical cell for observing solidification of helium. Cryogenics, 35, 71, (October 1995).

Adaptive-Grid Methods for Phase Field Models of Microstructure Development

PRINCIPAL INVESTIGATOR: Dr. Jonathan A. Dantzig

University of Illinois, Urbana-Champaign

CO-INVESTIGATORS:

Goldenfeld, N.

University of Illinois at Urbana-Champaign (UIUC)

Task Objective:

The objective of this newly-funded research program is to perform numerical studies of solidification to predict microstructure. Such calculations are currently limited by competing requirements for fine resolution at the interface and the need for including a sufficiently large domain to be physically meaningful. We will apply recently developed adaptive meshing algorithms capable of tracking solidification interfaces, along with the phase field model for phase transformations, to solve this computational problem.

Task Description:

We intend to examine pattern selection during phase transformations using adaptive meshing techniques. In these methods, we selectively refine a computational domain in the regions where higher precision is required, and leave the portions of the domain where relatively little variation occurs to be resolved on a coarser scale. These methods are ideally suited to this problem, where the large variations in the field variables are essentially confined to a very narrow region near the moving interface.

There are two key ideas in the application of adaptive mesh refinement. The first of these is a systematic means to determine where the mesh needs refinement through use of an estimator. The value of the error estimator in each element is used as a measure of the element's candidacy for local refinement or unrefinement. There are also important issues relating to the underlying data structure which space does not permit discussing here. The algorithms are referred to as {\it adaptive} because the mesh density is refined locally, based on the need for resolution.

The application of the adaptive mesh refinement scheme for the study of dendritic growth will be carried out in several steps. First, we will recast the phase field equations in finite element form, in order that we may use the error estimator that we have developed. We will consider the resolution of the nonlinear equations using a Newton-Raphson algorithm to improve convergence. It is critical to the success of this work that the algorithms be tested and compared with analytical solutions and published data wherever possible. To that end, we will consider several sample problems which are essentially one-dimensional. These include the growth of a sphere and a plane. Moving up in complexity, we will investigate the growth of small sinusoidal disturbances on a plane and check that the stability spectrum is accurately reproduced. Finally, we will check our algorithm on non-trivial structures by looking at the problem of melting, rather than solidification. In this case, a planar interface is stable, and we shall attempt to follow the backwards and stable evolution of an Ivantsov parabola into a plane. These tests will give us confidence that the adaptive grid method is computationally efficient and does not introduce any artifactual instabilities into the problem.

Task Significance:

Successful completion of this project will enable us for the first time to make accurate predictions of material microstructure under realistic growth conditions. The ability to do this is a necessary prerequisite for control and design of desired material properties. These results should also provide needed tests of theories for microstructure development, in conjunction with ongoing MSAD experimental programs.

Progress During FY 1996:

This is a new project this year, beginning in May. The objective of the project is to perform numerical studies of solidification to predict microstructure. We will use a phase field approach, in which the moving interface is replaced by a rapidly changing continuous function. This permits us to model the behavior on a fixed grid.

We have hired a postdoctoral research fellow, Dr. Nikolas Provatas, to work on the project. Dr. Provatas' previous research involved the application of phase field models to the study of flame front movement. He is therefore especially well qualified for the current program.

To date we have carefully studied the work of other researchers in the area, and have begun work on our adaptive gridding codes. The codes are being written in FORTRAN 90, in order to take advantage of the superior array handling and data manipulation capabilities of this language. At a later date, we expect to also take advantage of parallel solution algorithms being developed at other locations.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/96 **EXPIRATION:** 5/00**PROJECT IDENTIFICATION:** 962-21-05**NASA CONTRACT NO.:** NAG8-124**RESPONSIBLE CENTER:** MSFC

Atomistic Simulations of Cadmium Telluride: Toward Understanding the Benefits of Microgravity Crystal Growth

PRINCIPAL INVESTIGATOR: Dr. Jeffrey J. Derby

University of Minnesota

CO-INVESTIGATORS:

Chelikowsky, J.R.

University of Minnesota

Task Objective:

Progress in crystal growth on earth or in space will depend on a more fundamental understanding of the important coupling between atomistic-scale processes which control the properties of grown crystalline material and the macroscopic transport conditions imposed by the growth system. Our long-term goal is to understand the mechanisms which influence crystal quality through the hierarchy of length and time scales relevant to these atomistic-scale and macro-scale processes. The immediate goal of our research is to employ atomistic simulation to understand better the melt growth of cadmium telluride (CdTe) and its alloy cadmium zinc telluride (CdZnTe). These materials are employed in a variety of technologically important electronic and electro-optical devices; however, the growth of high-quality, large-area single crystal substrate has proven to be extremely difficult under terrestrial conditions. We seek to obtain a more fundamental understanding of the properties of cadmium telluride so that the physical mechanisms responsible for growth can be elucidated. A secondary objective of our work is the prediction of high-temperature thermophysical properties of liquid and solid CdTe.

Task Description:

For the studies described here, we will employ new *ab initio* pseudopotential codes for molecular dynamical simulations using quantum forces developed by Chelikowsky and co-workers. This technique has several advantages over traditional plane wave approaches. This scheme eliminates the fictitious electronic coordinates and finds a self-consistent solution at each time step in the molecular dynamics simulation. By constraining the evolution of the system to the Born-Oppenheimer surface, we may lengthen the time-step involved. Often the molecular dynamics time step can be increased by an order of magnitude or more. This compensates for the time increase from obtaining a self-consistent solution at each step. If one couples this with a Langevin molecular dynamics procedure, then the time step may be increased further as this type of dynamics does not require energy conservation at each step. Another advantage is that this procedure allows one to consider simulations in which the cell volume and shape change in a physical way with temperature and pressure. Since the system is constrained to reside on the Born-Oppenheimer surface, the interatomic forces are "true" forces. Also, insulating systems can be handled as well as metallic, or charged systems. We have successfully applied these techniques to liquid silicon and germanium, and current work is being carried out on liquid gallium arsenide and gallium phosphide. We foresee no problems in extending this work to CdTe.

Task Significance:

Recent growth experiments of $\text{Cd}_{0.96}\text{Zn}_{0.04}\text{Te}$ in a microgravity environment aboard USML-1 resulted in material which was far superior in structural perfection compared to earth-grown material under similar conditions. These dramatic results were attributed to the elimination of hydrostatic pressure from the melt column overlaying the crystal due to microgravity conditions, thereby reducing the hoop stresses that occur in a crystal as it grows and cools. In addition, it was speculated that the near absence of hydrostatic pressure allowed for the melt to solidify with minimal wall contact, thereby eliminating deleterious wall interactions. We will utilize atomistic simulation to understand the dynamics of the liquid/solid interface and of the solid material under the stress conditions corresponding to micro-gravity and terrestrial conditions. The work to be performed in this project will support current microgravity research on the melt growth of CdTe compounds and will provide for a quantitative, unambiguous method to understand the subtle effects of microgravity in these systems.

The primary thrust of this work will be to clarify the role of microgravity in interpreting the USML-1 results described above; however, this work promises to support future microgravity research in other substantial ways. Atomistic simulations will provide predictions of the high-temperature thermophysical properties of CdTe and its alloys. Accurate high-temperature properties are needed for reliable materials processing models, but such data are

extremely difficult to obtain from experimental measurements (many of which have been undertaken in microgravity environments). The prediction of these properties using atomistic simulation clearly complements ongoing and future microgravity process modeling and experimental property measurement efforts. Another likely benefit from this work is that a more complete understanding of the structure of molten CdTe and alloys will aid the development of seeding procedures for melt growth. For earth-based processes, reliable seeding techniques have not yet been developed for these materials, yet such procedures have been identified as one of the most needed process improvement to increase yields. Undoubtedly, as further microgravity experiments on the melt growth of CdZnTe are performed, seeded growth experiments will be desired and the knowledge obtained from atomistic simulations will be invaluable.

Progress During FY 1996:

This research program was funded starting April 1996, so only preliminary aspects of the program have gone forward in the past fiscal year. In the FY96 time frame, we have assigned a graduate student to the project and have defined the major technical issues of the work. Currently, our focus is on developing and testing interatomic potentials for cadmium and tellurium.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 4/96 **EXPIRATION:** 4/00

PROJECT IDENTIFICATION: 962-21-12

NASA CONTRACT No.: NAG8-125

RESPONSIBLE CENTER: MSFC

Use of Synchrotron White Beam X-ray Topography for the Characterization of the Microstructural Development of Crystal - Normal Gravity Versus Microgravity

PRINCIPAL INVESTIGATOR: Dr. Michael Dudley

State University of New York, Stony Brook

CO-INVESTIGATORS:

Larson, D.

State University of New York at Stony Brook

Task Objective:

The objective of the research proposed here is to provide an assessment of the influence of the accelerated cooling rates, imposed by severe limitations on available flight time, on the defect microstructure of crystals grown in a microgravity environment (using, for example, modified Bridgman or Vapor Transport techniques). Results previously obtained on ground-based ZnTe samples (grown by Vapor Transport at NASA Marshall Space Flight Center) seem to indicate that if cooling rates are too high the accentuated thermal mismatch stresses can give rise to deformation processes, comprising the formation of dislocation slip bands.

The objective of the present research is to extend the preliminary work on ground-based samples, to further ground-based samples, and also to flight samples grown with different cooling rates. The microstructures of the as-grown crystals will be non-destructively characterized using the technique of Synchrotron White Beam X-ray Topography (SWBXT). Correlations between the existence of significant post-growth deformation and accelerated growth rates will be directly examined.

The influence of accelerated cooling rates on the significance of the comparison drawn between normal gravity and microgravity crystal growth can thus be determined.

Task Description:

The research proposed here will be carried out using Synchrotron White Beam X-ray Topography (SWBXT) at the Stony Brook Synchrotron Topography Facility, which is under the direction of Prof. Dudley. It will consist of SWBXT characterization of crystals grown in a microgravity environment primarily obtained from co-investigator Dr. D.J. Larson, Jr., of Grumman Corporate Research Center, as well as from other sources such as Drs. D. Gillies and C.-H. Su at NASA Marshall Space Flight Center. Crystals of CdZnTe and ZnTe will be examined, although many other systems of interest to NASA are expected to be studied, for example ZnSe, CdTe, HgCdTe and PbSnSe. Opportunities will be sought amongst the NASA crystal growth community to maximize the amount of data obtained on as many different systems as possible. Crystals grown at various cooling rates will be examined, and the influence of these rates on the resulting microstructure will be assessed.

In the approach adopted here, reflection topographs from the cylindrical outside surface of the as-grown boules will be initially examined. These will provide information on the defect structures in the region from the outside surface down to the penetration depth of the x-ray beam, which is typically 5-10 μm . This enables an overall assessment of the distribution of defects such as twins, sub-grain and grain boundaries, and dislocations to be made. This can aid in the development of optimal wafering geometries to enable clearest visualization of the defect microstructure. Following this, both reflection and transmission topographs will be recorded from the individual wafers. Images obtained from the various wafers will be compared with those obtained from the original boules, and an overall representation of the three dimensional distribution of defects throughout the boule will thus be developed. By comparing such three dimensional representations of defects in crystals grown with various cooling rates, the influence of the cooling rate on the type and distribution of defects in the crystals can be determined.

It is anticipated that results may indicate that accelerated cooling rates, dictated by schedule limitations, have a dominant effect on the microstructure of crystals grown in a microgravity environment, thus obscuring information on the influence of the magnitude of the gravity vector. It is further anticipated that these results may lead to a change in the criteria used to determine time allocation for individual crystal growth experiments on future flights in order to avoid effects on crystal microstructure resulting from effects unrelated to the magnitude of the gravity vector.

Task Significance:

Much effort has been, and continues to be, expended by NASA in evaluating the influence of a microgravity environment on the defect microstructures developed in crystals during crystal growth. While the influence of a microgravity environment on crystal growth is generally accepted as being beneficial, it is not clear that prior studies of this influence have been unperturbed by artifacts related to the particular choice of experimental conditions. Indeed, in order to properly compare crystal growth in a microgravity environment to that in a normal gravity environment it is important to be able to isolate the influence exerted by the difference in magnitude of the gravity vector on the resultant crystal quality. Effects associated with accelerated cooling rates, or sudden changes in temperature gradient, imposed either deliberately or inadvertently, detract from the significance of such experiments. Results already obtained from ZnTe crystals grown in a normal gravity environment seem to indicate that stresses generated by thermal mismatch effects during cooling can significantly affect the observed, as-grown defect microstructure. These stresses lead to the formation of dislocation slip bands which tend to obscure and/or break up the true growth defect microstructure. Should such effects occur in crystals grown in a microgravity environment, the true influence of microgravity on crystal quality cannot be assessed.

It is thus of paramount importance to be able to assess the effect of the accelerated cooling rates, dictated by flight schedule limitations, on resulting defect microstructures. One can gain insight into the chronological history of the development of the final defect microstructure from analysis of images recorded using Synchrotron White Beam X-ray Topography (SWBXT). This is a non-destructive imaging diffraction technique capable of revealing the detailed defect microstructure in large single crystals. Such defect microstructures in crystals grown with various cooling rates will be compared and examined for evidence of extensive, post-growth slip. Maximum usable cooling rates can thus be determined.

Determination of the influence of cooling rate on the defect microstructure of crystals is crucial for selection of experimental conditions under which the effects of the gravity vector on crystal growth quality can be usefully investigated. Once such selection has been optimized, differences in microstructure observed in microgravity grown crystals may be safely attributed to the influence of the gravity vector, and not to artifacts related to compressed growth schedules.

Should accelerated cooling rates be shown to have a detrimental effect on defect microstructures in microgravity grown crystals, it is likely that this result could modify the criteria used to determine the experimental schedules for microgravity crystal growth.

Progress During FY 1996:

Systematic investigation of defect structures in all the wafers sliced from the two CdZnTe flight samples (GCRC 1 and 2) grown during the First United States Microgravity Laboratory Mission (USML-1) revealed that the crystalline quality of as-grown crystals is strongly influenced by both the accelerated cooling rate and the occurrence of wall contact.

In GCRC 1, x-ray topographs recorded from the gradient freeze growth regions (both rapid and changing cooling rate) show highly distorted images, indicating that this region is heavily strained. It is believed that very large axial thermal stresses can be generated by the large axial temperature gradient imposed by the rapid cooling process leading to severe deformation processes. The solidification rate of the steady-state growth region is ten times lower than that of gradient-freeze growth. The effect of accelerated cooling rates to the crystalline quality is clearly revealed by the difference in defect structures. In steady-state growth region, no significant lattice distortions are observed. The most prominent structural defect comprises of two sets of long, straight asymmetrically distributed small angle tilt boundaries nucleated near the ampoule wall and propagating into the interior of the wafer along the crystallographic 10^{-1} and $0^{-1}1$ directions.

In GCRC 2, x-ray topographic observations revealed that the density of dislocations increased significantly as the cooling rate was accelerated. In order to investigate the distribution and density of dislocations, a wafer was thinned down to a thickness of less than 180 microns for transmission studies. Transmission x-ray topographs recorded from steady-state growth regions revealed that the dislocation density is approximately $10^3/\text{cm}^2$ (this is three orders of magnitude smaller than the best ground-based samples). This result is in good agreement with etch pit density (EPD) studies, in which a dislocation density of approximately $800/\text{cm}^2$ in the best region was obtained, while in the gradient freeze region (near the tail end of the wafer), a very high dislocation density was observed. Since the

density of dislocations is just about at the resolution limit of the technique, a dislocation density of approximately 10^5 - $10^6/\text{cm}^2$ can be determined.

X-ray topographic studies also revealed that the crystalline quality of as-grown crystals can be strongly influenced by wall contact. In GCRC 2, regions of very high structural perfection are observed from the portion of the crystal solidified without wall contact, while a pronounced twin structure is evident in wall contact regions. Systematic investigation of the distribution of twins in all the ten wafers sliced from GCRC 2 enabled one to reconstruct the twin configuration in this boule. All twins were nucleated from the wall contact, shoulder region and propagated through the boule during crystal growth. The twinned region occupies approximately 35 percent of the crystal volume. In addition, an individual grain, nucleated from the wall contact region, separated from a twin oriented region by a curved, high angle grain boundary is also observed. This indicates that the magnitude of stresses associated with wall contact can be very large, giving rise to the formation of a single grain. In the matrix, which is solidified without wall contact, neither the formation of twins nor slip bands is observed; only several small angle tilt boundaries confined at the periphery can be discerned. In addition, dislocations also appeared to be concentrated in twin oriented regions where a well defined dislocation mosaic structure was observed. In contrast, regions of very low dislocation density were observed in the matrix. Dislocation mosaic structures in CdZnTe crystals can be generated during the post solidification cooling process under the influence of thermal gradient induced stresses (S. Mcdevitt *et al.*, Mater. Lett., 4, p 451 (1986)). Since the twins are produced during growth, they are created before the generation of the dislocation mosaic structures, and they also may act as barriers to the propagation of dislocations.

In melt growth, the temperature gradients imposed during solidification and cooling processes may induce thermal stresses leading to the formation of dislocations if the resolved shear stress is larger than the critical resolved shear stress (CRSS) of the material at the growth temperature. X-ray topographs recorded from GCRC 2 revealed that the density of dislocations increased significantly as the cooling rate was accelerated. In addition, the highly distorted image recorded from gradient freeze regions in GCRC 1 strongly suggested the occurrence of severe deformation processes. It is, therefore, expected that large thermal stresses can be generated by the rapid cooling processes imposed by constrained space flight schedules giving rise to dislocation generation. In addition, due to different thermal properties between CdZnTe and the quartz ampoules, significant thermal stress can be generated at the peripheral region of a boule during this rapid cooling process. Although lattice hardening can be achieved by doping of CdTe with Zn (R. S. Rai *et al.*, J. Vac. Sci. Technol., B9, p 1892 (1991)), the nucleation of extensive slip bands was still observed in the flight samples. This result is evidence of the formation of large stresses in the peripheral regions of crystal during growth. Thermo-mechanical stress simulations of flight experiments indicated that a dramatic increase in local stresses can occur if adhesion between the growing crystal and the ampoule wall occurred (D. J. Larson *et al.*, Proc. of the SPIE, 2228, p 11 (1994)). It is, therefore, expected that the magnitude of stresses associated with rapid cooling can be amplified by effects associated with wall contact. This could give rise to the occurrence of the type of extensive plastic deformation process observed in the flight samples.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/94 **EXPIRATION:** 7/97

PROJECT IDENTIFICATION: 962-21-08-27

NASA CONTRACT NO.: NCC8-048

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Chung, H., Raghothamachar, B., Wu, J., Dudley, M., Larson, Jr., D.J., and Gillies, D.C. "Characterization of Growth Defects in CdZnTe Single Crystals by Synchrotron White Beam X-ray Topography, in "Defect and Impurity-Engineered Semiconductors and Devices" (S. Ahok, J. Chevallier, I. Akasaki, N.M. Johnson, and B.L. Sopori, Eds.)." Mat. Res. Soc. Symp. Proc., 378, 41-46 (1995).

Dudley, M., Larson Jr., D.J., Chung, H., and Raghothamachar, B. "Characterization of Zn-Alloyed CdTe Compound Semiconductors Processed in Microgravity on USML-1 and USML-2." Proceedings of 31st COSPAR Scientific Assembly, Birmingham, United Kingdom, July 14-21, 1996 ("Advances in Space Research").

Larson Jr., D.J., Dudley, M., Chung, H., and Raghothamachar, B. "Synchrotron Characterization of Zn-Alloyed CdTe Compound Semiconductors Processed in Microgravity on STS-50 and STS-73." IUCR Proceedings (1996).

Combined Synchrotron White Beam X-Ray Topography and High Resolution Triple Axis X-Ray Diffraction Characterization and Analysis of Crystals Grown in Microgravity and Ground Based Experiments

PRINCIPAL INVESTIGATOR: Dr. Michael Dudley

State University of New York, Stony Brook

CO-INVESTIGATORS:

Matyi, R.J.

University of Wisconsin at Madison

Task Objective:

Among the most important issues in any bulk crystal growth process is the reduction of the density of grown-in structural defects and the understanding of the relation between crystal growth and defect generation. The quantitative analysis of defects in semiconductor single crystals is typically complicated by the difficulty in separating the effects from various structural defects. Typically, semiconductor crystals contain a variety of defects; the effects of these structural defects are usually convolved together, making it difficult to quantitatively assess the concentrations of a specific defect type in a particular sample or to unambiguously relate a given defect to the crystal growth conditions.

The objective of the research proposed here is to carry out detailed studies of defect and general distortion distributions in crystals grown in both microgravity and ground-based environments (using, for example, modified Bridgman or Vapor Transport techniques) using a combination of synchrotron white beam X-ray topography (SWBXT) and high resolution triple crystal X-ray diffractometry (HRTXD). This unique combination of techniques is expected to reveal detailed differences between crystals grown in these two different environments and to enable a meaningful assessment to be made of the influence of a microgravity environment on various aspects of the quality of crystals grown therein. SWBXT and HRTXD are complementary analytical techniques which are most sensitive and useful at contrasting ends of the "scale" of defect densities in semiconductor crystals. By applying both techniques to the same crystals, it will be possible to provide detailed and quantitative assessments of the defect structure from regions that range from highly perfect (where SWBXT is expected to be the superior characterization tool) to highly imperfect (where HRTXD should be the superior method). This unified and continuous view of the defect structure should lead to valuable insights into the effect of growth conditions on the defect generation process.

The proposed research program will draw upon the extensive experience that has been gained at the State University of New York-Stony Brook and University of Wisconsin-Madison in the analysis of defects in semiconductors using advanced methods of X-ray diffraction. Prof. Michael Dudley of SUNY-Stony Brook has worked closely with the crystal growth community at NASA's Marshall Space Flight Center in applying methods of SWBXT to numerous semiconductor crystals grown both on earth and in microgravity. His counterpart, Prof. Richard Matyi of University of Wisconsin, Madison, has been actively engaged in demonstrating the capabilities of HRTXD to a variety of semiconductor materials. By combining these complementary techniques it should be possible to obtain a deeper understanding of the process of defect generation than would be possible with either technique alone, or perhaps by any structural probe.

Task Description:

A complete description will be sought of the type and distribution of all defects present in the crystals to be examined. Crystals will initially be examined in boule form using both SWBXT and HRTXD in reflection geometry in order to reveal the overall distribution of defects and distortion around the cylindrical surface of the crystal. This will help determine the optimal wafering geometry to be adopted for the next stage of the research. Once the boules have been suitably wafered, SWBXT and HRTXD will be used, in sequence, to examine the defect and distortion distributions in each of the wafers. Information so gathered will then be compiled to reconstruct complete three dimensional defect and distortion distributions in the as-grown boule. This reconstructed information can then be used to compare with the predictions of growth models. A preliminary attempt at the latter has already been published.

The central problems in characterizing grown-in defects in single crystals which are to be addressed in this research are: (a) how does one distinguish between different defects that may be present in a crystal? (b) can quantitative measurements be made to assess the density of any one defect type? (c) can this information be related back to the crystal growth process in order to both understand the impact on growth parameters on defect generation and to reduce the grown-in defect density for improved crystal quality? These issues are especially pertinent to the analysis of crystals grown in a microgravity environment, where significant expenditures of both time and money are made in order to grow crystals which can test theories of fluid flow and may lead to properties that are superior to those attainable in ground-based laboratories. If microgravity crystal growth is to be used to elucidate the fundamental scientific issues of microstructure evolution, then it is desirable to have the most advanced characterization capabilities developed in order to both qualitatively and quantitatively demonstrate the beneficial aspects of microgravity crystal growth. Furthermore, in order to properly compare crystal growth in a microgravity environment to that in a ground-based gravity environment it is important to be able to isolate the significance of the difference in magnitude of the gravity vector. Effects associated with accelerated cooling rates, or sudden changes in temperature gradient, imposed either deliberately or inadvertently, detract from the significance of such experiments. Results already obtained from ZnTe crystals grown in a ground-based gravity environment and from CdZnTe crystals grown in both ground-based and microgravity environments seem to indicate that stresses generated by thermal mismatch effects during cooling can significantly affect the observed, as-grown defect microstructure. This research, commenced under NRA-93-OSSA-12 will be continued as part of this research program.

In this research program, the evolution of crystal growth defects in bulk compound semiconductors will be examined in a variety of semiconductor crystals grown under approved flight experiments on USML-2 and USMP-3. We will examine crystals that range from a relatively high degree of structural perfection (Ge and GaAs) through those where a larger defect density is anticipated (CdZnTe, HgZnTe and HgCdTe) down to crystals where a very high defect density is expected (PbSnTe). Moreover, we will examine corresponding samples of these crystals grown on earth as a function of crystal growth conditions and relate the nature and quantity of these defects to the crystal growth process. In particular, the influence of cooling rate on the microstructure of crystals grown in both microgravity and ground-based environments will be examined. This work will confirm that the crystals were grown under circumstances which enable the useful assessment of the influence of the magnitude of the gravity vector on the quality of crystals grown.

The four year program involves the application of x-ray diffraction methods for characterization of II-VI semiconductors grown in microgravity. There are three specific goals for this program: (1) demonstration of the coordinated use of white beam synchrotron topography and high resolution triple axis diffractometry as complementary tools for the quantitative analyses of structural defects in semiconductor crystals; (2) the application of these X-ray analytical methods to compound semiconductor crystals (grown both in ground-based experiments and in microgravity) to achieve a better understanding of the effects of the crystal growth environment on the generation of defects; and, (3) creation of a feedback loop to the Space Science Laboratory (SSL) at MSFC to incorporate these results into future growth experiments.

Task Significance:

The central hypothesis of this research is that the combined use of two complementary methods of x-ray diffraction analysis -- synchrotron white beam x-ray topography (SWBXT) and high resolution triple crystal x-ray diffractometry (HRTXD) -- can yield new insights into the mechanism of crystal growth and the process of defect generation during growth. The fact that SWBXT is expected to be a superior method for defect characterization when the defect density is low, while HRTXD is expected to be superior at high defect densities, means that the two techniques can be used in concert to quantitatively analyze a large range of crystal defect structures. We believe that the information gained from the synergistic application of these two characterization methods to the same materials will result in an improved understanding of the effects of microgravity on crystal growth.

The significance of the research described here is that it will directly determine the influence of a microgravity environment on the detailed defect and distortion distribution in crystals produced in flight experiments, and will enable direct comparison to be drawn with crystals produced in ground-based experiments. Confirmation will be obtained that effects resulting from the limited flight times available for microgravity crystal growth experiments do not exert control over the microstructure of the crystals grown, potentially detracting from the intended assessment of the influence of the magnitude of the gravity vector on these processes. Determination of the influence of cooling rate on the defect microstructure of crystals is crucial for selection of experimental conditions under which the effects of the gravity vector on crystal growth quality can be usefully investigated. Once such selection has

been optimized, differences in microstructure observed in microgravity grown crystals may be safely attributed to the influence of the gravity vector and not to artifacts related to compressed growth schedules.

Progress During FY 1996:

Preliminary results have been obtained from six crystal boules: a ZnTe boule, sliced into wafers, grown by Dr. D. Gillies at NASA Marshall Space Flight Center (MSFC); two CdZnTe boules, examined as-grown and following wafering, grown on USML-1, by Dr. D.J. Larson, at Grumman Corporate Research Center; a ground-based CdZnTe boule, again grown by Dr. Larson, and two ground-based ZnSe boules grown by Dr. C.-H. Su at MSFC. In the wafers from the ZnTe boule, Synchrotron White Beam X-ray Topography (SWBXT) revealed a detailed twinning structure and the presence of a cellular dislocation structure comprising small angle subgrain boundaries with relatively low dislocation density existing within the subgrains. High Resolution Triple Axis Diffraction HRTXD experiments on the same ZnTe sample yields reciprocal space maps consisting of multiple surface streaks; behavior which is characteristic of a sample with large mosaic blocks that are relatively perfect (low in dislocation density) but with a high degree of misorientation with respect to each other. This interpretation is in agreement with the topographic observations of the same material described above.

SWBXT of CdZnTe crystals grown on USML-1 reveal areas of very low defect density (with individual dislocations being resolvable as well as precipitates) when the cooling rate is low. When slices from the more rapidly cooled regions of the boule are examined, higher dislocation densities and extensive slip become apparent. These results confirm the initial hypothesis that accelerated cooling rates, imposed by compressed flight schedules, can obscure and/or destroy the underlying actual growth defect structure, hindering the assessment of the influence of gravity vector magnitude on crystal quality. In general it appears that increasing cooling rate first increases the overall growth dislocation density, and then produces slip which obscures this growth defect structure. This appears to be in general agreement with earlier observations. Further work in this area is underway and is envisaged in this program. HRTXD studies of same CdZnTe samples grown on USML-1 reveal a well-defined crystal truncation rod, or surface streak, which extends perpendicular to the surface. This feature, which arises from the fact that the crystal surface truncates the bulk lattice, contains the dynamically diffracted intensity from the bulk crystal. The presence of a well-defined surface streak is indicative of two qualities of the diffracting crystal: (1) the bulk crystal has sufficient structural perfection in order to diffract dynamically, and (2) the crystal surface is of high enough quality to produce the surface streak at all. It should be noted, however, that the surface streak in this sample is less intense than is typically seen in samples of highly perfect Ge or GaAs; this degradation is likely to be due to the grown-in dislocation density in this sample. This interpretation is supported by the diffuse intensity located off the surface streak in the vicinity of the 333 reciprocal lattice point. The roughly symmetric distribution of diffuse intensity about the 333 point is indicative of a relatively isotropic distribution of dislocations in the diffracting volume. Overall the agreement between SWBXT and HRTXD results is very good.

Reciprocal space maps from two different ZnSe samples grown at MSFC by Dr. C.-H. Su, when recorded from a cleaved (110) surface and showed a well-defined surface streak. The large amount of diffuse scatter evident indicates a high dislocation density; however, the uniformity of the diffuse intensity suggests that the dislocations are randomly distributed throughout the crystal and not concentrated into subgrain boundaries. Lattice maps recorded from ZnSe samples with a polished surface reveal the absence of any surface streak and both the intensity and the angular extent of the diffuse intensity indicates a highly defective surface region in this sample. This interpretation also agrees with observations from a SWBXT of the same samples, thus supporting our belief in the complementary nature of the two characterization techniques.

In order to establish a quantitative link between the two techniques, we have developed a theoretical framework for calculating the effect of dislocations in bulk II-VI semiconductors on the diffuse x-ray scattering observed in high resolution triple crystal x-ray diffraction (HRTXD) measurements. In this approach we have adopted a model based in the kinematical theory for straight dislocations in which the Burgers vector is parallel to the $\langle 110 \rangle$ directions. The calculated diffuse scattering profile perpendicular to a reciprocal lattice vector has been compared with experimental intensity profiles recorded from the (333) reflection from CdZnTe and the (220) reflection from ZnSe. In the case of the CdZnTe, good agreement between the theoretical and experimental scattering curves were obtained for an assumed dislocation density in the range of $1\text{E}+05\text{ cm}^{-2}$, while the ZnSe scattering profile was adequately fit with assumed density of $2\text{E}+07\text{ cm}^{-2}$. We are currently working on refining this model through comparison with synchrotron topography data.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 1

PhD Students: 1

TASK INITIATION: 4/96 EXPIRATION: 4/97

PROJECT IDENTIFICATION: 962-21-13

NASA CONTRACT No.: NCC8-93

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Chung, H., Raghothamachar, B., Dudley, M., and Larson, Jr., D.J. "Synchrotron White Beam X-Ray Topography Characterization of Structural Defects in Microgravity and Ground Based CdZnTe crystals (in "Space Processing of Materials")." SPIE Proceedings, vol. 2809, 45-56 (1996).

Chung, H., Raghothamachar, B., Zhou, W., Dudley, M., and Gillies, D.C. "Studies of Interface Demarcation and Structural Defects in Ga doped Ge Single Crystals by Synchrotron White Beam X-Ray Topography (in "Applications of Synchrotron Radiation to Materials Science," L. Terminello, S. Mini, D. L. Perry, and H. Ade, eds.)." Mat. Res. Soc. Symp. Proc., 437 (1996).

Reverse Micelle Based Synthesis of Microporous Materials in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Prabir K. Dutta

Ohio State University

CO-INVESTIGATORS:

Kresge, C.T.
Ansari, R.Mobil Research and Development
NASA Lewis Research Center (LeRC)

Task Objective:

The objective of this program is to develop a better understanding of nucleation and crystal growth of microporous materials. The mechanisms underlying crystal growth are complicated because of the heterogeneity of the reactant composition. This has made it difficult to determine the chemical features that are responsible for the crystal framework as well as its morphology. Yet, without definite identify and control of these features, microporous material synthesis will continue to be dominated by a trial and error approach. Conventional spectroscopic probes have had difficulty in identifying the relevant precursors.

Task Description:

Conventional microporous materials are made by hydrothermal synthesis. Considerable research is being done in evaluating the basic chemistry involved in the synthesis. We have developed a new method that uses microdroplets of water (reverse micelles) in an oil-like medium as the site for nucleation. This process allows us to examine particle growth by laser light scattering. In addition, control of the distribution of reactants within the reverse micelles leads to various crystal growth pathways. Our focus at present is to expand the types of frameworks that can be grown by this method. We are also investigating the role of hydrogen ions in the crystallization process as well as the influence of cations that are introduced via the detergent in making the reverse micelles. Adapting the knowledge gained from reverse micelle synthesis to more conventional and widely practiced hydrothermal synthesis of aluminosilicates is essential. We have begun this process by investigating the time scale involved in the nucleation process. Also, alteration of crystallization pathways by modulating the thermal input into the reaction system is being investigated. Ultimately, our goal is to design procedures that will benefit from microgravity because of lack of sedimentation and convection, leading to crystal growth under very special conditions. This is so for the reverse micelle based process, since particle size increases gradually with time and leads to sedimentation, thus resulting in arrested crystal growth.

Task Significance:

Microporous materials play a very important role in many technologies. Ion-exchange properties of these materials are exploited in the manufacture of detergents. The microporosity and acidity of these solids play a key role in many chemical and petrochemical industries, including the production of gasoline and starting materials for commonly used polymers. Brand new technologies have developed because of the synthesis of new frameworks. Our contributions in understanding the basic molecular events that are responsible for formation of microporous materials should lead to more directed synthesis of novel framework structures.

Progress During FY 1996:

In 1995, we reported the first synthesis of a microporous material using reactants enclosed in reverse micelles (Nature 374, 44, 1995). A complete account of the crystallization process in these systems has just been published in 1996. It showed that reverse micelles, by virtue of their ability to exchange the contents of the water pools, resulted in considerable control over crystallization pathways. Currently, we have been exploring if frameworks other than the zincophosphate sodalite can be made in reverse micelles. This would extend the scope of this methodology. Results have however been discouraging. All attempts to grow faujasite-like framework have been unsuccessful. However, we are finding that this is arising because of the strong structure-directing effect of the cation that is present as a result of the surfactant used to make the reverse micelle. Efforts are underway to minimize the cation effect by using selective complexing agents such as crown ethers. We are also understanding the role of the cation in the synthesis process.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/96 EXPIRATION: 5/97

PROJECT IDENTIFICATION: 962-21-27

NASA CONTRACT No.: NAG8-126

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Reddy, K.S.N., Salvati, L.M., Dutta, P.K., Abel, P.B., Suh, K.I., and Ansari, R.R. Reverse Micelle Based Growth of Zincophosphate Sodalite: Examination of Crystal Growth. J. of Physical Chem., vol. 100, 9870-9880 (1996).

Reverse Micelle Based Synthesis of Microporous Materials in Microgravity

PRINCIPAL INVESTIGATOR: Prof. Prabir K. Dutta

Ohio State University

CO-INVESTIGATORS:

Kresge, D.T.

Mobil Research & Development Corporation

Ansari, R.

NASA Lewis Research Center (LeRC)

Meyer, W.

NASA Lewis Research Center (LeRC)

Task Objective:

The objective of this research is to better understand the synthesis of microporous materials, especially those based on a network of connecting substructures. Examples of microporous materials include zeolites which are widely used as catalysts and absorbents.

Task Description:

The synthesis of zincophosphate microporous material is studied via a novel synthesis route using reverse micelles. The reverse micelles isolate small portions of reactant and allow examination of mechanism of crystal formation. The crystal growth processes are studied to determine the influence of convective flows and Stokes setting. Conditions for zincophosphate growth appropriate for an orbit experimentation are being identified.

Task Significance:

Microporous materials have extremely wide application as catalysts and absorbents. Their complex structure is derived from chemical and physical transformations which have to date eluded investigators. This research separates portions of the nucleation and growth process for examinations. It is leading to a greater understanding of how these materials form, to new synthesis routes, and eventually to new materials and thereby to changes in economics of technologies, such as petroleum processing.

Progress During FY 1996:

We have investigated in detail the three pathways reported in 1995. The reverse micelle is providing the control on supersaturation by minor changes in intramicellar reactant composition, as evidenced from the NMR data. In composition A, where the supersaturation is the lowest, crystal growth proceeds slowly, controlled by surface attachment kinetics. Atomic force microscopy and scanning electron microscopy support this conclusion. The growth process in Pathway B can be analyzed as an aggregation process. The early morphology of these crystals is similar to that of composition A, and further growth occurs by diffusion-controlled micellar collisions. In pathway C, the intramicellar conditions result in higher supersaturation, which leads to rapid nucleation, and since the induction time for crystal formation is longer, amorphous particles are formed. These particles age, and are covered by solvent water, where nucleation begins. Such a mechanism is supported by the rotating cell experiment, in which suspended amorphous particles were found to directly transform to sodalite crystals. The most important conclusion from this study is that reverse micelles allow for control of crystal growth. Minimal sedimentation and convection in microgravity will allow us to examine the complete crystal growth process for these different pathways.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 0

PhD Students: 1

TASK INITIATION: 1/93 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 963-26-05-01

NASA CONTRACT NO.: NAG3-141

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Reddy, K.S.N., Salvati, L.M., Dutta, P.K., Abel, P.B., Suh, K.I., and Ansari, R.R., Reverse micelle based growth of zincophosphate sodalite: examination of crystal growth. *Journal of Physical Chemistry*, 100, 9870-9880 (1996).

Studies on Nucleation, Polymerization, and Nanoparticle Composites in Supersaturated Vapors under Microgravity Conditions

PRINCIPAL INVESTIGATOR: Dr. M. S. El-Shall

Virginia Commonwealth University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The general objective of the ground-based experiments is to advance the scientific understanding of nucleation and materials synthesis from the vapor phase which are strongly influenced by gravity and convection effects. These experiments will provide insights into the fundamental aspects of nucleation and related materials processes and will eventually lead to cloud chamber experiments on nucleation, gas phase polymerization and nanoparticle synthesis in a high quality, long duration, microgravity environment. Our specific objectives in this research are:

1. Development of new methods for the study of ion nucleation on well-defined ions in supersaturated vapors.
2. Development of gas phase ionic polymerization by laser induced initiation in supersaturated vapors using nucleation as a detector for the growing polymer molecules.
3. Synthesis of nanoscale composite particles with controlled size and compositions by combining laser vaporization of metals with controlled condensation in a diffusion cloud chamber.

Task Description:

The overall four-year research plan includes experiments on nucleation, gas phase polymerization and nanoparticle composites. A new technique is being developed for the study of nucleation on well-defined ions. The method is based on Resonance Ionization, in which well-defined molecular ions act as nucleation centers for the condensation of supersaturated vapors. These experiments allow, for the first time, to selectively and unambiguously generate specific ions of interest and study their nucleating behaviors during the condensation of supersaturated vapors.

The study of gas phase polymerization is conducted within supersaturated monomer vapors in diffusion cloud chambers. Polymerization is initiated by multi-photon ionization of the monomer molecules or by generating metal cations within the vapor phase.

The nanoparticle composites are prepared by combining pulsed laser vaporization of metal targets with controlled condensation from the vapor phase. The use of laser vaporization combined with olefin polymerization will lead to the synthesis of polymers containing ultrafine metal particles which could have novel properties.

Task Significance:

This research will provide detailed understanding of nucleation, gas phase polymerization, and nanoscale particles. Nucleation is one of the most ubiquitous and important phenomena in science and technology. It plays a central role in materials science, crystal growth, chemical processing, atmospheric science and cosmochemistry. The study of gas phase polymerization is an important intellectual and technological frontier in which promises unique results not only for a fundamental understanding of polymerization reactions, but also for the development of new materials with unique properties. In the past it has been almost impossible to study gas phase polymerization because the involatile product molecules condensed out of the gas phase. Nanoscale particles possess several unique properties such as large surface areas, unusual adsorptive properties, surface defects and fast diffusivities. The control and characterization of these properties can ultimately lead to identifying many potential uses, particularly in the fields of catalysis and novel materials. This research will develop new methods to study gas phase polymerization and nanoscale particles under a microgravity environment which is expected to allow the design of novel cluster engineered materials with tailored unique properties.

Progress During FY 1996:

We have demonstrated the application of resonance enhanced multiphoton ionization (REMPI) to selectively and unambiguously generate molecular ions of interest and study their nucleating behaviors in supersaturated host vapors. We have also investigated the effect of carrier gas pressure on the measurements of homogeneous nucleation rates in diffusion cloud chambers. At higher pressures, convection and chamber instability can limit the measurements of nucleation rates. Model calculations are in progress in order to predict the optimum operating conditions of the cloud chamber under microgravity.

We have prepared several nanoparticles by using a laser vaporization-controlled condensation technique from the vapor phase. The optical and luminescence properties of these particles have been investigated. Current work is concerned with incorporating these particles in different polymeric films and studying their optical properties.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 2

TASK INITIATION: 5/96 EXPIRATION: 4/00

PROJECT IDENTIFICATION: 962-21-46

NASA CONTRACT NO.: NAG8-127

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Kane, D.B., and El-Shall, M.S. Condensation of supersaturated vapors of hydrogen bonding molecules: ethylene glycol, propylene glycol, trimethylene glycol and glycerol. J. Chem. Phys., vol. 105, 7617-7632 (1996).

Kane, D.B., and El-Shall, M.S. Ion nucleation as a detector: application of REMPI to generate selected ions in supersaturated vapors. Chem. Phys. Letters, vol. 259, 482-487 (1996).

Presentations

El-Shall, M.S. "Studies on nucleation, polymerization, and nanoparticle composites in supersaturated vapors under microgravity." NASA Microgravity Materials Science Conference, Huntsville, Alabama, June 10-12, 1996.

El-Shall, M.S. "From clusters to polymers and nanoparticles: a route to novel materials." 70th American Chemical Society Colloid and Surface Science Symposium, Clarkson University, Potsdam, New York, June 16-19, 1996.

El-Shall, M.S. "Surface oxidation and luminescence properties of weblike agglomeration of silicon nanocrystals produced by a laser vaporization - controlled condensation technique." Fifth Annual Meeting of the Consortium for Nanostructured Materials, Vanderbilt University, Nashville, Tennessee, October 18-19, 1996.

Kane, D.B., Fisenko, S.P., and El-Shall, M.S. "Pressure effect on nucleation rate measurements in diffusion cloud chambers." Fourteenth International Conference on Nucleation and Atmospheric Aerosols, Helsinki, Finland, August 26-30, 1996.

Theoretical and Experimental Investigation of Vibrational Control of the Bridgman Crystal Growth Technique

PRINCIPAL INVESTIGATOR: Dr. Alexandre I. Fedoseyev

University of Alabama, Huntsville

CO-INVESTIGATORS:

Alexander, J.I.D.

University of Alabama-Huntsville (UAH)

Task Objective:

The primary objectives are to:

- 1) conduct a parametric theoretical and numerical investigation of vibro-convective buoyancy-driven flow in differentially heated cylindrical containers;
- 2) investigate buoyant vibro-convective transport regimes in Bridgman-type systems with a focus on the use of vibration to suppress, or control, convection in order to achieve transport control during crystal growth;
- 3) assess the feasibility of vibro-convective control as a means of offsetting "g-jitter" effects under microgravity conditions; and,
- 4) exchange information with the experimental group at the General Physics Institute (GPI) of the Russian Academy of Science who are undertaking a complementary experimental program.

Task Description:

The proposed research will involve a numerical investigation of vibro-convective transport regimes with application to the control of convection and transport during growth of crystal by the Bridgman technique.

The basic problems to be analyzed will be the suppression or control of buoyancy-driven convection in melts during plane-front directional solidification. The work will involve the analysis of vibrational interaction with natural convection and its effects on the temporal evolution of melt temperature and composition during growth. The philosophy behind our approach is to use numerical modeling in two ways: synergistically with experimental developments, and as a predictive tool. The synergism-with-experimentation will allow careful interpretation of both experimental and modeling results for what can be a highly non-linear physical situation. By exploring regimes and system properties currently inaccessible to experimentation, the model can also be used as a predictive tool. The work will involve an extensive investigation of the vibrational flow regimes with and without the presence of natural buoyancy-driven convection and will be initially guided by previous results. As we progress toward our goal of defining the applicability of vibrational control of convection we will compare the ability of vibration to suppress flow with that of a magnetic field and also explore the consequences of using simultaneous vibration and magnetic field control.

Task Significance:

The character of natural buoyant convection in rigidly contained inhomogeneous fluids can be drastically altered by vibration of the container boundaries or through the introduction of vibration sources into the interior of the fluid.

Control of convective transport continues to be an important aspect of crystal growth research. Control of convection through static and rotating magnetic fields is being actively pursued by several groups. However, there are many instances, whether due to materials properties or other practical considerations, in which use of magnetic fields to induce stirring or suppress flow may not be an option. In such cases, vibrational control could become an attractive alternative.

While active vibration isolation can be a partial solution, it will not solve the problems that might arise due to the quasi-steady and very low-frequency acceleration components related to the gravity gradient and other orbital factors. Thus as an alternative to vibration isolation, one might envisage using vibration to either suppress flow or to provide flow regimes tailored to particular crystal growth experiments. These flows would not be accessible under

terrestrial conditions due to strong natural convection effects. Thus, the microgravity relevance of our proposed work is established.

Progress During FY 1996:

Funding started in June 1996. Since then we have, following consultation with our colleagues at the General Physics Institute (GPI) in Moscow, chosen two models systems. The first involves only thermovibrational convection with no consideration of solidification. Our calculations will be performed synergistically with flow visualization experiments at the GPI. The second system will involve directional solidification of a two-component alloy crystal.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 6/97

PROJECT IDENTIFICATION: 962-21-14

NASA CONTRACT No.: NAG8-122

RESPONSIBLE CENTER: MSFC

The Impaction, Spreading, and Solidification of a Partially Solidified Undercooled Drop

PRINCIPAL INVESTIGATOR: Dr. Merton C. Flemings

Massachusetts Institute of Technology (MIT)

CO-INVESTIGATORS:

Trapaga, G.

Massachusetts Institute of Technology (MIT)

Task Objective:

The purpose of this project is to examine the spreading of molten metal droplets and their solidification upon impacting onto a solid cooled surface.

Task Description:

This project is aimed at studying the splatting and solidification behavior of undercooled and partially solidified metallic specimens. The project consists of both an experimental component and a computational and analytical component.

In the experimental arrangement, a levitated and inductively melted metallic droplet is allowed to fall in the Marshall Space Flight Center drop tube, cool during flight and then impinge on a chilled solid substrate. The flattening process is recorded using high speed photography and the resulting splats are subsequently collected and analyzed. The thermal management of the system is arranged so that upon approaching the chilled substrate, the droplets are undercooled in the range of 10° - 500°C ; although for some control experiments, we impinge either superheated droplets or droplets close to their melting temperature. Additionally, a number of experiments are carried out such that undercooled droplets are made to impinge on the flat surface of a room temperature substrate.

The theoretical work includes the development of a new set of equations to describe the behavior of the partially solidified droplet upon impact and the calculation of the velocity and rate of cooling of the specimen as it falls. In addition, we address issues of impingement and splatting under conditions where the viscosity of the undercooled materials does not necessarily follow Newtonian behavior. Different kinds of materials are considered in this investigation to cover a wide range of melting temperatures and sample viscosities.

Task Significance:

The problem of the spreading and solidification of molten metal droplets is of both fundamental and practical interest. The fundamental interest is provided by the fact that the simultaneous spreading and solidification of metal droplets is a generic problem in materials processing. The practical interest is associated with the immediate relevance of these phenomena to spray forming and the formation of coatings.

Progress During FY 1996:

Two sets of experimental campaigns were performed using NASA's unique tower facility at the Marshall Space Flight Center and employing an extensive range of materials. The experiments were performed in collaboration with NASA personnel and researchers from Caltech.

The experimental component of the project was combined with a theoretical part in which computer simulations were employed to better understand the spreading/solidification process and to establish the conditions required to design such experiments. In addition, an experimental campaign was carried out using the experimental facilities available at MIT to compare the behavior of spreading droplets under different conditions to those at the Marshall facility (i.e., very low relative U_i as well as much lower degrees of undercooling). The main accomplishments during this period include the demonstration of the experimental approach to produce splats of different materials and the large number of recordings of splattings obtained using state of the art high speed photography. Data analysis and comparison between experimental data and predictions were also performed.

The combined experimental and theoretical work performed during this period has allowed for the planning of a new experimental campaign that will take place at the end of October at the Marshall facility. During these experiments, high speed cameras will be used to simultaneously record the evolution of the spreading process (i.e., diameter and height vs. time), as well the instantaneous temperature history for a wide range of materials, including pure metals,

deep eutectics and glass-forming metals. These materials will be dropped on a transparent substrate to allow measurements of temperature from the bottom of the spreading samples, while the spreading process will be recorded from lateral views at 45 degrees from the impingement point.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	1
PhD Students:	0	PhD Degrees:	0

TASK INITIATION: 9/94 **EXPIRATION:** 9/96**PROJECT IDENTIFICATION:** 962-25-08-35**RESPONSIBLE CENTER:** MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Schwenke, G.K. "Analysis of the Non-Isothermal Impact Spreading and Freezing of Metal Droplets." MIT MS Thesis (June 1996).

Investigation of Local Effects on Microstructure Evolution

PRINCIPAL INVESTIGATOR: Dr. Donald O. Frazier

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Rogers, J.

NASA Marshall Space Flight Center (MSFC)

Downey, P.

NASA Marshall Space Flight Center (MSFC)

Facemire, B.

NASA Marshall Space Flight Center (MSFC)

Witherow, B.

NASA Marshall Space Flight Center (MSFC)

Task Objective:

The objective of this proposed work is to perform modeling and experimental studies on the development of microstructures and the growth of a second phase in a two-phase system. Most modeling and experimental studies focus on the average particle and the late stages of growth processes. However, experimental observations of dynamic local behaviors within the context of a particle ensemble are accessible by optical techniques, including holography. Interest extends to examining these systems in all stages of growth within the limit of holographic resolution. Additionally, holography provides and archives data to employ emerging techniques for measuring diffusion fields during growth.

Task Description:

The primary method of data collection is by the use of holography. The holographic techniques are crucial to capturing the entire cell volume. A unique capability to apply phase shifting interferometry to holography is under development by one of the co-investigators of this work. With this technique it is possible to measure the concentration gradients, hence diffusion fields, surrounding individual droplets. Such data, not attainable by any other techniques, would provide essential input to computer models. Additionally, a two-color holography technique, also under development by the same co-investigator, may provide measurement of spurious thermal gradients over the lifetime of an experiment. It should be noted that use of narrow path-length cells can introduce the effects of "mixed" dimensionality, as observed in recent analysis of an experiment performed in this laboratory. "Mixed" dimensionality refers to 3-D droplets located on a 2-D substrate. Such systems follow different scaling laws than fully 3-D systems.

The research approach includes observation of diffusional growth of the secondary phase in a transparent monotectic system. Ultimately, this work will rely on the benefits of microgravity processing to eliminate the buoyancy caused by concentration or temperature gradients. Ground work requires a transparent isopycnic system. Sensitivity to gravitational fields is tested, in the laboratory, by tethering two droplets in a test cell and comparing growth kinetics at varying temperatures. Convective flows increase with increasing conjugate phase density differences which are relatively strong functions of temperature. Quench experiments in narrow path-length cells allow observation of local effects in an ensemble of droplets. Narrow path-length is a prerequisite for establishing transparency quickly in high droplet density media.

Task Significance:

To a large extent, particle growth and distribution determine the mechanical properties of an alloy. An understanding of microstructure is essential to predicting the behavior of a material with respect to, for example, metal fatigue. The unique capabilities provided by holographic techniques enabling observations of local effects during diffusional growth of a second phase in a model transparent two-phase system allows detailed analyses of the local dynamic and resulting microstructures. Additionally, holographic studies of droplet diffusion in model systems are in agreement with Rutherford backscattering measurements of Ga and Sn "island" growth on Si. Likewise, cloud dynamics derives some of its physics from such coarsening phenomena. Diffusional studies to model the time evolution of the total surface area of particles comprising polar stratospheric clouds, for example, suspected as catalysts for ozone decomposition, can be potentially important to the study of the rate of ozone layer depletion.

Progress During FY 1996:

The multipole model that introduces concentration gradient asymmetries effectively eliminates non-ideal long range interactions between particles. A screening phenomenon analogous to the Debye-Huckel screening in ionic solutions occurs. The mass flux of any given droplet feels the influence of near-neighbors; hence a droplet beyond a given cluster should sense a deviation in growth kinetics expected in the absence of screening (low droplet volume fraction). In our investigation in collaboration with Rensselaer Polytechnic Institute (RPI) and the Naval Research Laboratory (NRL) on the role of dipole terms in the description of three-dimensional coarsening we have demonstrated that at volume fractions above $\approx 1\%$ consideration of dipole terms is important in accounting for deviations from the ideal LSW model.

Additionally, we suggest a new approach to the study of Ostwald ripening among a finite cluster of precipitates in liquid-liquid systems. The concept identifies spatial instabilities and self-structuring within an initially homogeneous arrangement of a finite number of droplets with accompanying experimental and numerical methods. Development of the concept begins with manual measurements of the positions and sizes of droplets obtained from holographic images. Image analysis incorporates finite-cluster coarsening theory, and proceeds with software development for visualization of the calculated diffusion fluxes and their spatial correlation.

The volume of potential data points begs for development of automated image analysis and user-friendly software to facilitate a necessarily statistical approach to these tasks. Recent progress has accelerated input to the development of a proposal to continue this work.

STUDENTS FUNDED UNDER RESEARCH:**TASK INITIATION:** 6/94 **EXPIRATION:** 6/96**PROJECT IDENTIFICATION:** 962-26-08-13**NASA CONTRACT No.:** NCC8-054**RESPONSIBLE CENTER:** MSFC

Melt Stabilization of PbSnTe in a Magnetic Field

PRINCIPAL INVESTIGATOR: Dr. Archibald L. Fripp

NASA Langley Research Center (LaRC)

CO-INVESTIGATORS:

Debnam, W.J.

NASA Langley Research Center (LaRC)

Rosch, W.R.

National Research Council at NASA Langley

Szofran, F.R.

NASA Marshall Space Flight Center (MSFC)

Chait, A.

NASA Lewis Research Center (LeRC)

Yao, M.

Ohio AeroSpace Institute

Task Objective:

The objective of this research is to further elucidate the gravity driven physical phenomena on the growth of the alloy compound semiconductor, PbSnTe. The effect of the gravitational body force on the convective properties of the alloy compound semiconductor, PbSnTe, with that body force modified by both reduced gravity and by magnetohydrodynamic (MHD) damping, is the subject under investigation. PbSnTe is an ideal material for this study in that it was the material of a 1996 AADSF experiment and another experiment to take place in 1997. Both of these experiments are without magnetic fields. Subsequent experiments using MHD damping, both ground-based and in space, will form a complete set of experiments that will further elucidate the gravity dependent physical phenomena on the growth of this class of materials.

Task Description:

The application of a magnetic field to PbSnTe growth will dampen convective flow. The anticipated results are that even in the MSFC superconducting magnet furnace the growth will not become diffusion controlled but that the combination of magnetic field and low gravity environment will produce diffusion controlled growth.

Numerical modeling is an integral part of this endeavor. Computer simulation can aid in the design of the space experiment by its predictive capacity to optimize conditions for the growth. The key purposes of this portion of the study will be to optimize the growth for both Earth and the space experiments and to obtain an estimate of the required magnetic field strength for low gravity growth.

Task Significance:

This work, along with magnetic-field low-gravity experiments to be proposed, will complete the set. It will compare the effects of convection, as modified by a magnetic field, on the growth of this material both on Earth and in the microgravity environment found in low Earth orbit. This work, coupled with the past microgravity experiment with the MEA and the existing flight program to grow PbSnTe in the AADSF, will form the most comprehensive set of space processing experiments performed to date.

Progress During FY 1996:

The ground-based experiments are relatively straightforward: crystals are grown in a magnetic field. After growth they are evaluated for compositional uniformity and defect structure. The experimental parameters are ampoule dimensions, temperature gradient, and magnetic field strength and orientation. The solutal driving force can be varied by both changing the growth rate, the temperature gradient, ampoule size, and by changing the starting ratio of SnTe to PbTe. Numerical analysis helps select the experimental matrix.

Experimental results to date of 1 cm diameter crystals grown in a 80 °C/cm thermal gradient with growth rate as a parameter are indistinguishable from the totally mixed results obtained without magnetic fields, even with the 5T field. This result, for these conditions, was predicted by our numerical analysis.

The flight experiment to be proposed will simulate that of the AADSF experiment but with the addition of the stabilizing magnetic field. Depending on further study, a specific Shuttle attitude may be requested for growth such that the crystal is grown with the ampoule axis aligned with the steady state gravity vector.

The primary objectives of the numerical analysis portion of this effort are to provide a quantitative understanding of the complex transport phenomena during solidification of non-dilute binaries (such as PbSnTe), to furnish a numerical tool for furnace design and growth condition optimization, to provide estimates of the required magnetic field strength for low gravity growth, and to assess the role of magnetic damping for space and ground control of the double-diffusive convection. The modeling and solution procedure established previously will be largely retained and refined as the work continues.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-21-23

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Yao, M., Chait, A., Fripp, A.L., and Debnam, W.J. Numerical Simulation of Bridgman Crystal Growth of PbSnTe in Microgravity. Microgravity Science and Technology, vol. 8, 214 (1995).

Solidification of II-VI Compounds in a Rotating Magnetic Field

PRINCIPAL INVESTIGATOR: Dr. Donald C. Gillies

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Benz, K.W.

University of Freiburg, Germany

Volz, M.P.

NASA Marshall Space Flight Center (MSFC)

Mazuruk, K.

Universities Space Research Association (USRA)

Task Objective:

The primary aim of this work is to study the effects of a rotating magnetic field (RMF) on solidification, and especially how it affects crystal growth. The RMF gives rise to a rotational or stirring effect in the liquid column. The principal geometry to be studied is that found in the traveling heater method (THM). In this case there is a small zone of constant dimensions and aspect ratio. In addition, during growth the thermal field and the composition field will remain reasonably constant. The program will initially be ground-based, and as such will encompass several types of experiments and several different materials. Studies of flow in a cell specially designed to emulate a THM zone or a float zone will be used to test the effect of field strength and frequency on the flow induced by an applied RMF. In particular, the interaction of the field with buoyancy driven flow, and the transition from laminar to turbulent flow will be investigated, both by test cell measurements and by modeling.

Task Description:

The first task will be to examine the effects of a rotating magnetic field of varying field strength and frequency on the flow induced in a test cell containing gallium. The primary aim will be to study the flow and determine how the magnetically induced flow interacts with the natural gravity produced buoyancy. This will give us a data base with which we can test computer simulations. These models will then be fine tuned and applied to the crystal growth configurations of interest.

Secondly, the intention is to establish the criteria for accelerated controlled growth of this class of materials by the traveling heater method. This will include modeling, and the measurement of several of the important and unknown thermophysical constants. These include electrical and thermal conductivity of the solvent zone compositions for Te-HgCdTe, Te-HgZnTe, Te-CdTe, Te-CdZnTe and Te-CdTeSe systems. Viscosity and its variation with temperature will also be measured on these materials. These results will be incorporated into the models.

On earth selected samples will be grown both with and without the application of the rotating magnetic field. These experiments will be tailored to determine the effects of the fluid flow during solidification. Extensive characterization will be performed aimed at determining the distribution of the alloying elements, the presence and distribution of defects, the control of inclusions and precipitates, with the ultimate aim of determining how the solidification history is influenced by fluid flow.

A fluid cell, probably including gallium, capable of operation in a microgravity glove box will be constructed. Such a unit will be miniaturized and will operate within a rotating magnetic field. The data obtainable by any subsequent orbital experiment will give vital information on the effect of the RMF unperturbed by buoyancy effects and will enable the study of different regimes, and the testing of theories of behavior of flow in a RMF to be made.

Task Significance:

The proposed study will establish the usefulness of the rotating magnetic field as a viable method of crystal growth. The principal advantage of the method is the enhancement of control of fluid flow during solidification both on the ground and in space. Such control has the potential for realizing several different regimes of solidification in complex alloys, particularly pseudo-binary II-VI compounds. In the traveling heater method the increase in flux transport achievable through controlled flow with the magnetic field has the potential to save considerable time for what is normally the slowest of bulk crystal growth techniques. The removal of the boundary layer will alleviate instability problems. A long term aim is the production of small quantities of high quality material from long duration flight experiments in microgravity. This will lead to a better knowledge of the fundamental parameters of an important class of materials which are difficult to grow on earth.

Progress During FY 1996:

This is the first year of the project, and the main progress so far has been two-fold. On the theoretical side, modeling of the THM unit has been initiated. This initial modeling has been a thermal model and has aided in designing and scaling the zone fabrication for the THM furnaces, and the dimensions of the magnets. The design of the equipment is almost complete. It is anticipated that the first growth of HgCdTe samples will take place early next year.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 4/96 EXPIRATION: 4/99

PROJECT IDENTIFICATION: 962-21-15

RESPONSIBLE CENTER: MSFC

Electronic Materials

PRINCIPAL INVESTIGATOR: Mr. Thomas K. Glasgow

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

Duval, W.M.B.

NASA Lewis Research Center (LeRC)

Nelson, E.S.

NASA Lewis Research Center (LeRC)

Rogers, R.

NASA Lewis Research Center (LeRC)

Task Objective:

The major objective of this task is to provide monitoring of a number of ground-based research projects performed in academia. The task also supports some ground-based laboratory facilities and a limited research program, particularly in the areas of mixing driven by steady and time variant acceleration, salt solidification, and physical vapor transport.

Task Description:

The phenomena being studied include diffusion, coarsening, solution crystal growth, physical vapor transport, pattern formation in solidification of aggregation, solute rejection and transport, and nucleation behavior. The gravitational acceleration considered ranges from constant 1-g low and variable g-levels (g-jitter).

Task Significance:

The important feature of this work is the coordinated approach; i.e., quantitative agreement is sought between physical and numerical experiments. Attention must therefore be given to the development of diagnostic tools as well as to advanced numerical techniques.

Progress During FY 1996:

Under this task we cover the monitoring of numerous ground-based investigations. An in house task has provided support for the examination of g-jitter effects. The influence of residual acceleration on microgravity experiments continues to be a matter of concern.

The task has supported technology transfer for Stereo Imaging Velocimetry and Surface Light Scattering. SIV has been used by LTV Steel to better understand flow in the continuous casting process. SLS has been demonstrated at Containerless Research Inc. and is now part of their NRA supported research.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/92 EXPIRATION: N.A.

BS Students: 3

PROJECT IDENTIFICATION: 962-21-05-02

MS Students: 1

NASA CONTRACT NO.: None

PhD Students: 0

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Kim, G.T., Lin, J.T., Jones, O.C., Glicksman, M.F., Duval, W.M.B., Singh, N.B., Effects of convection during the physical vapor transport process: application of laser doppler velocimetry. *Journal of Crystal Growth*, (in press, 1996).

Singh, N.B., Glicksman, M.F., Coriell, S.R., Duval, W.M.B., Santoro, G.J., Dewitt, R., Measurement of diffusion coefficient using a diaphragm cell: PbBr₂-AgBr. *Journal of Crystal Growth*, (in press, 1996).

Zhou, A., Zebis, A., Trivedi, S., Duval, W.M.B., Physical vapor transport of zinc-telluride by dissociative sublimation. *Journal of Crystal Growth*, (in press, 1996).

Presentations

Duval, W.M.B., "Flow field topology of buoyancy induced mixing." AIAA-96-0253, 34th Aerospace Sciences Meeting & Exhibit, Reno, NV., January 15-18, 1996.

Effect of Gravity on the Evolution of Spatial Arrangement of Features in Microstructure: A Quantitative Approach

PRINCIPAL INVESTIGATOR: Prof. Arun M. Gokhale

Georgia Institute of Technology

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

1. To develop the quantitative microscopic techniques for the characterization of spatial arrangement of features in microstructures by using digital image analysis and Stereology.
2. To apply the new methodology to quantify the evolution of spatial arrangement of tungsten grains during liquid phase sintering of a series of tungsten heavy alloys.
3. To quantify the role of gravity in the evolution of spatial arrangement of tungsten grains during liquid phase sintering of tungsten heavy alloys.

Task Description:

Digital image analysis and stereological procedures will be developed for quantitative characterization of the spatial arrangement of features in microstructural space. The serial microstructure and computer simulations of three-dimensional microstructures will also be utilized to develop these techniques. The methodology will be applied to quantify the evolution of the spatial arrangement of tungsten grains in the liquid phase sintered specimens of tungsten heavy alloys, processed by Professor R.M. German. The quantitative characterization of similar specimens processed in a microgravity environment will permit analysis of the effect of gravity on the evolution of the spatial arrangement of microstructural features.

Task Significance:

It is well known that the spatial arrangement of features have a pronounced effect on material properties and performance. The spatial arrangement of microstructural features is governed by the intrinsic microstructural evolution processes and gravity. The methodology developed in this research, and the quantitative data on the evolution of spatial arrangement of tungsten grains during liquid phase sintering, should be very useful to understanding the effect of intrinsic materials processes on the evolution of spatial distribution of microstructural features, and to quantify the role of Earth's gravity in the microstructural evolution.

Progress During FY 1996:

Specimens of liquid phase sintered tungsten heavy alloys have been obtained from Professor R.M. German at Pennsylvania State University. These specimens were processed in microgravity in an earlier space flight experiment of Professor German. A detailed microstructural analysis of these specimens is under progress. We are particularly interested in quantitatively characterizing the evolution of the spatial arrangement of tungsten grains during liquid phase sintering process, and the effect of gravity on this aspect of microstructural evolution. For this purpose the digital image analysis procedure developed earlier for creation of a "montage" of a large number of contiguous microstructural fields is being utilized. This procedure is applied to measure centroids of a large number of features in the microstructural montage. A separate computer code is developed for calculating the spatial distribution functions that describe the spatial arrangement of features in a metallographic plane. These techniques are being applied for quantitative characterization of the evolution of the spatial arrangement of tungsten grains during liquid phase sintering in a series of tungsten heavy alloys processed on Earth as well as in microgravity. The resulting data will be analyzed to gauge the contribution of Earth's gravity in dictating the evolution of spatial arrangement of grains during liquid phase sintering.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 2

PhD Students: 0

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-21-36

NASA CONTRACT NO.: NAG8-124

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Tewari, A., and Gokhale, A.M. "Evolution of Microstructural Distance Distributions During Liquid Phase Sintering in Normal Gravity and Microgravity." NASA Microgravity Materials Science Conference, Huntsville, Alabama, June 10-12, 1996.

Evolution of Microstructural Distance Distributions in Normal Gravity and Microgravity

PRINCIPAL INVESTIGATOR: Prof. Arun M. Gokhale

Georgia Institute of Technology

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

1. To develop the methodology for estimation of distribution of distances between microstructural features by using digital image analysis and stereological techniques.
2. To apply the methodology to quantify the evolution of microstructural distance distributions during liquid phase Sintering.
3. To gauge the role of Earth's gravity in the evolution of microstructural spatial distance distributions.

Task Description:

Digital image analysis techniques will be applied to obtain the relative locations of microstructural features observed in metallographic planes in the specimens of liquid has sintered tungsten heavy alloys. These data will be utilized to calculate the radial distribution function and the pair correlation functions of tungsten grains. The quantitative information will be used to monitor the evolution of spatial distribution of tungsten grains during liquid phase sintering in the normal gravity and microgravity.

Task Significance:

An important effect of Earth's gravity on the microstructural kinetics is through its influence on the spatial arrangement of features in microstructure. This research program will develop the techniques for quantitative characterization of the evolution of microstructural distance distributions during materials processes. The results should be useful to gauge the relative contributions of intrinsic materials processes and gravity on the evolution of the spatial arrangement of features in microstructure.

Progress During FY 1996:

Interactive software was used to create a "montage" of a large number of microstructural fields in the memory of the image analyzing computer. The software removes the "edge effect" problems associated with individual microstructural fields, and permits measurements of centroid coordinates and sizes of a larger number of microstructural features in a series of microstructural fields. Software codes have been developed to extract the statistical descriptors of the spatial arrangement of the microstructural features, such as radial distribution function and pair correlation function. These procedures have been applied to quantify the evolution of the spatial distribution of tungsten grains in the liquid phase sintered specimens of WHA alloys processed on Earth and in the microgravity environment. These specimens were provided by Professor R.M. German of Pennsylvania State University. The experimental data on the evolution of spatial distance distributions are utilized to gauge the effect of Earth's gravity on the microstructural evolution during liquid phase sintering.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 0

TASK INITIATION: 7/94 EXPIRATION: 7/96

PROJECT IDENTIFICATION: 962-25-05-29

NASA CONTRACT NO.: NAG3-165

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Pascal, L., and Gokhale, A.M., Computer simulation of spatial arrangement and connectivity of features in three-dimensional microstructure: application to model electrical conductivity of polymer matrix composite. Acta Metallurgica et Materialia, vol. 44, pp 1519-1528 (1996).

Presentations

Tewari, A. and Gokhale, A.M., "Evolution of microstructural distance distributions during liquid phase sintering in normal gravity and microgravity." Microgravity Materials Science Conference, organized by NASA., Huntsville, Alabama, June 10-12, 1996.

Plasma Dust Crystallization

PRINCIPAL INVESTIGATOR: Dr. John A. Goree

University of Iowa

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to demonstrate that charged particulates in a plasma environment form an ordered structure.

Task Description:

The investigator will design and test apparatus for radio-frequency (RF) plasma generation/particulate confinement, and analyze the structure of suspended particulates. This will include working with German scientists in designing microgravity experiments.

Task Significance:

This investigation begins a new genre of microgravity research. It will provide (1) a macroscopic model of how atoms arrange themselves in a crystal or liquid, (2) a much-needed test of dusty plasma theories used in space physics and astronomy, and (3) an understanding of particulate contamination during plasma processing steps of microchip manufacturing.

Progress During FY 1996:

A series of ground-based experiments was undertaken to advance and exploit our new plasma crystal technique. The plasma crystal consists of plastic microspheres that are charged and levitated in a gas discharge plasma. They arrange themselves in ordered structures. We produced and studied crystalline lattices, fluids near the freezing point, isotropic fluids, gases, and the hexatic intermediate phase that lies between the crystalline and liquid phases of 2-dimensional media.

Analysis methods and hardware were tested in the laboratory to define concepts for future flight experiments. As collaborators for a DARA-funded German experiment that is planned as a get-away-special, we advised in the design of the flight hardware.

Theoretical simulations were carried out to characterize the inter-particle potentials for the microspheres in the plasma.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	1
PhD Students:	3	PhD Degrees:	0

TASK INITIATION: 4/93 EXPIRATION: 4/96

PROJECT IDENTIFICATION: 963-25-10

NASA CONTRACT NO.: NAG8-292

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Melands, F., and Goree, J. Particle Simulation of Two-Dimensional Dust Crystal Formation. J. of Vacuum Science and Tech. A, vol. 14, 519- 524 (1996).

Melandso, F., and Goree, J. Polarized Supersonic Plasma Flow Simulation for Charged Bodies such as Dust Particles and Spacecraft. Physical Review E, vol. 52, 5312-5326 (1995).

Pieper, J.B., Goree, J., and Quinn, R.A. Experimental Studies of 2D and 3D Structure in a Crystallized Dusty Plasma. J. of Vacuum Science and Tech. A, vol. 14, 511- 518 (1996).

Praburam, G., and Goree, J. Sensitivity of the Scattering Ratio Method for Sizing Sub-Micron Particles Suspended in a Plasma. *Plasma Sources Science and Tech.*, vol. 5, 84-92 (1996).

Praburam, G., and Goree, J. Evolution of a Particulate Cloud in an RF Plasma. *IEEE Transactions on Plasma Science*, vol. 24, 97-98 (1996).

Praburam, G., and Goree, J. Experimental Observation of Very Low-Frequency Macroscopic Modes in a Dusty Plasma. *Physics of Plasmas*, vol. 3, 1212-1219 (1996).

Quinn, R.A., Cui, C.S., Goree, J., Pieper, J.B., Thomas, H., and Morfill, G. Structural Analysis of a Coulomb Lattice in a Dusty Plasma. *Physical Review E*, vol. 53, 53-56 (1996).

Presentations

Goree, J. "Dynamics of a Carbon Particle Cloud in a Sputtering Plasma." Workshop on Dusty Plasmas 1995, Wickenburg, Arizona, October 1995.

Goree, J. "Plasma Dust Crystallization." NASA Fluid Physics Microgravity Conference, Cleveland, Ohio, June 1996.

Goree, J., and Pieper, J.B. "Experiments with Strongly-Coupled Dusty Plasmas." Workshop on Dusty Plasmas 1995, Wickenburg, Arizona, October 1995.

Goree, J., and Pieper, J.B. "Experiments with Strongly-Coupled Dusty Plasmas." Gaseous Electronics Conference, Berkeley, California, October 1995.

Goree, J., and Pieper, J.B. "Experiments with Strongly-Coupled Dusty Plasmas." American Physical Society, March Meeting, St. Louis, Missouri, March 1996.

Utilizing Controlled Vibrations in a Microgravity Environment to Understand and Promote Microstructural Homogeneity during Floating-Zone Crystal Growth

PRINCIPAL INVESTIGATOR: Dr. Richard N. Grugel

Universities Space Research Association (USRA)

CO-INVESTIGATORS:

Wang, T.G.

Vanderbilt University

Anilkumar, A.V.

Vanderbilt University

Hurd, J.L.

IBM

Croll, A.

Albert-Ludwigs University (Freiburg, Germany)

Task Objective:

Crystal quality should improve during float-zone processing if inherent convective flow within the liquid volume can be minimized. Consequently, the objective of this experimental and theoretical investigation is to utilize vibration driven surface streaming flows in an effort to negate the detrimental effects of thermocapillary convection which arise during float-zoning of semiconductor materials. The processing parameters will be evaluated with the intent of optimizing microstructural homogeneity. This ground-based work will then be extended to the microgravity environment where the effect of thermocapillary flow on crystal homogeneity may be studied in an optimized floating-zone.

Task Description:

The ground-based experimental and theoretical work will concentrate on defining the role various processing parameters play in promoting microstructural uniformity during floating-zone crystal growth. In particular, float-zone dimensions, aspect ratios, oscillation frequency, and amplitude will be evaluated with the intent of understanding how thermocapillary flow is negated. To this end, work has already been initiated by utilizing the transparent sodium nitrate - barium nitrate model system; further insight regarding crystal homogeneity will be gained by processing sodium nitrate crystals which have been doped with silver nitrate.

Task Significance:

Gravity driven flow which occurs during float-zone processing is minimized in a microgravity environment and thus permits thermocapillary flow to be singularly investigated. Here, utilizing incremented and calibrated vibration, the consequence of flow velocities on microstructure can be controlled and systematically investigated, not just acknowledged. The microgravity environment will minimize unit-gravity induced biases such as static shape distortion and buoyancy flow; furthermore, sedimentation of tracer particles will be minimized. Here then is an opportunity to evaluate crystal growth and homogeneity in association with a stable and dimensionally optimized floating-zone. The results of this study could well demonstrate a novel and inexpensive way of considerably improving crystal uniformity.

Progress During FY 1996:

Work has just been initiated. A Ph.D. candidate, Mr. Paul Lemaster of Vanderbilt University, has been selected. Prof. Vladimir Sennitski from the Lavrentyev Institute of Hydrodynamics has arrived and will be working out of the University of Alabama at Huntsville (six or twelve months) as a Visiting Scholar. He will use his theoretical expertise to complement the experimental aspects of the ground-based experiments. Crystals previously grown are presently being evaluated at the IBM Research Laboratory.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 0

PhD Students: 1

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-21-16

NASA CONTRACT NO.: NCC8-66

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Shen, X.F., Anilkumar, A.V., Grugel, R.N., and Wang, T.G. Utilizing vibration to promote microstructural homogeneity during floating-zone crystal growth processing. *J. Cryst. Growth*, vol. 165, 438-446 (1996).

Presentations

Grugel, R.N. "Utilizing Controlled Vibrations in a Microgravity Environment to Understand and Promote Microstructural Homogeneity During Floating-zone Crystal Growth (poster presentation)." Microgravity Materials Science Conference. Huntsville, Alabama, June 10-11, 1996.

Novel Directional Solidification Processing of Hypermonotectic Alloys

PRINCIPAL INVESTIGATOR: Dr. Richard N. Grugel

Universities Space Research Association (USRA)

CO-INVESTIGATORS:

Alexander, J.I.D.

University of Alabama at Huntsville (UAH)

Task Objective:

The investigation has several scientific objectives which will be realized by conducting a systematic experimental investigation in conjunction with a thorough modeling effort. The theoretical study will develop a semi-quantitative predictive model relating microstructure to process parameters for the systems investigated experimentally. This will require close interaction with the experiment in order to determine more precisely the role of the various dynamic processes induced by ultrasound in these monotectic systems. Experimentally, ultrasound will be utilized to suspend and maintain separation of the Liquid II droplets which precipitate from the bulk once the temperature drops below the miscibility gap boundary so that a uniformly aligned hypermonotectic composite might actually be produced by controlled directional solidification.

Task Description:

The systematic, controlled directional solidification, experimental investigation will utilize a series of alloy compositions ranging from the monotectic reaction to well into the miscibility gap. Two sample sets will be investigated, one in conjunction with ultrasonics and one, otherwise identically processed, without. Metallographic examination will provide information regarding phase spacings, phase distributions, and volume fractions. The model will pay particular attention to the nature of the ultrasonic waves, including reflection and refraction of longitudinal waves and the 2-liquid phase boundary, and on the importance of standing waves. Evaluation of the model and analysis of the data will provide valuable guidelines for optimizing a microgravity experiment.

Task Significance:

Subsequent examination of the processed samples will promote our understanding of diffusion and coalescence processes, liquid-liquid interactions, wetting phenomena, and microstructural development. The liquid volume fraction ultrasonics can maintain dispersed versus the coalescing (settling) force imposed by gravity will be determined and then evaluated whether or not this could be improved upon in a microgravity environment. The value of this work will be a demonstration and mathematical characterization of a novel solidification processing technique. The knowledge acquired from investigating model alloys might then be applied to technologically relevant miscibility gap systems (e.g., superconducting Cu-Ba-Y), with the potential of producing novel composites having improved properties.

Progress During FY 1996:

Work has just begun. Research furnaces previously used by the PI at Vanderbilt University have been installed within the Space Science Laboratory and some initial experiments have been conducted. Prof. Vladimir Sennitski from the Lavrentyev Institute of Hydrodynamics has arrived and will be working out of the University of Alabama at Huntsville (six or twelve months) as a Visiting Scholar. He will use his theoretical expertise to complement the experimental aspects of the ground-based experiments.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-21-37

NASA CONTRACT NO.: NCC8-66

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Grugel, R.N. "Novel Directional Solidification Processing of Hypermonotectic Alloys (poster presentation)." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Influence of Free Convection in Dissolution

PRINCIPAL INVESTIGATOR: Prof. Prabhat K. Gupta

Ohio State University

CO-INVESTIGATORS:

Korpela, S.A.

Ohio State University

Task Objective:

To study the influence of natural convection in dissolution of silica glass into a melt consisting of PbO and SiO_2 .

Task Description:

The following two part task has been undertaken. One portion consists of designing an experiment to measure the composition profiles as a function of time and temperature of dissolution. The other part involves the design of a computer program for theoretical calculations.

Task Significance:

Dissolution plays an important role in processing of materials and in their use. Examples include corrosion of containers for molten slags and glasses, and dissolution of materials in liquid environments at room and low temperatures. The aim of this research is to provide a detailed understanding of the influence of free convection in the dissolution kinetics of solids in corrosive liquids by developing a theoretical model and using numerical analysis techniques to solve the model using computers in order to describe the results of ground based experiments of dissolution kinetics in simple binary systems.

Progress During FY 1996:

Isothermal dissolution of pure silica glass in lead metasilicate melts (50 mole % PbO -50% SiO_2) is being studied at several different temperatures in the range 750 to 850 C. To avoid the cracking due to thermal stresses caused by a large difference in the thermal expansion coefficients of the two phases upon cooling to the room temperature, a configuration was chosen where the melt is contained in a thin silica tube. Electron microprobe analysis is being carried out to measure the radial composition profiles as a function of vertical distance, time and temperature of dissolution. A computer program has been written to solve the fundamental equations for the case of large Schmidt numbers describing the dissolution of a semi-infinite vertical plate in a semi-infinite viscous melt in presence of free convection. Steady state solutions have been obtained and transient solutions are being worked on numerically.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 6/94 EXPIRATION: 8/97

PROJECT IDENTIFICATION: 962-25-05-24

NASA CONTRACT No.: NAG3-160

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Ainsworth, P.J. and Gupta, P.K. "Influence of free convection in dissolution." Annual meeting of the American Ceramics Society, Indianapolis, IN 1996, Ceramic Bulletin, 75, p267.

Microgravity Processing of Oxide Superconductors

PRINCIPAL INVESTIGATOR: Dr. William H. Hofmeister

Vanderbilt University

CO-INVESTIGATORS:

Bayuzick, R.J.

Vanderbilt University

Singh, N.B.

Westinghouse S&TC

Vlasse, M.

NASA Marshall Space Flight Center (MSFC)

McCallum, R.W.

Iowa State University

Task Objective:

Since the discovery of superconductivity in lanthanide-based perovskite systems, considerable effort has concentrated on the synthesis and characterization of these materials. Melt processing techniques have shown great promise in developing bulk crystalline materials with critical current densities necessary for practical application. The YBaCuO system has received the most intense study, as this material has shown promise for the application of both thin film and bulk materials. However, little information is available on the complete melting relations, undercooling, and solidification behavior of these materials. In general, the understanding of undercooling and solidification of high temperature oxide systems lags behind the science of these phenomena in metallic systems. Therefore, this research will investigate the fundamental melting relations, undercooling, and solidification behavior of oxide superconductors through melt processing, with an emphasis on improving ground-based synthesis of these materials. The techniques developed by this project will apply to oxide superconductors in general and will provide additional avenues for research in this field. An additional goal of this program is to develop collaboration with other groups and provide access to the unique processing strategies developed by the microgravity program.

Task Description:

The proposed research will continue experiments with $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$ using drop tubes at Vanderbilt University, the 105 meter drop tube at MSFC, and aero-acoustic levitation at Containerless Research, Inc. Microstructural and compositional analyses will be performed at Vanderbilt University and the Marshall Space Flight Center. Application of acoustic levitation and microwave heating at JPL, electrostatic levitation at JPL, undercooling combined with rapid heat removal in the URQT drop tube at Vanderbilt, and addition of small amounts of Ag to the material for improving electromagnetic susceptibility, will be explored and incorporated if the techniques prove useful. Also, rare-earth substituted 1:2:3 will be processed in order to decrease the melting temperature and ease melting. In order to correctly assess thermal profiles upon melting and solidification in aero-acoustic levitation experiments, the ultra high speed thermal imager (UHSTI) at Vanderbilt University will be utilized.

Task Significance:

Since the discovery of high- T_c superconductivity in copper oxide systems, much progress has been made in the area of thin film technology for small scale applications. However, the science suffers from the lack of crystalline materials with high critical current densities that are large enough for bulk or large scale applications. Melt processing in general has proven to be the best technique for producing bulk materials with significant critical current densities ($<10^4$ amp cm^{-2} in melt texturing experiments).

The novel techniques developed in this study have brought new insight into the understanding of the phase relations in this complex system. These enhancements will help to advance the understanding of the science of high- T_c superconductivity and of the material properties of oxide superconductors. Advancements have a direct impact on the production of bulk materials for large scale applications.

Progress During FY 1996:

Investigations utilizing aero-acoustic levitation (AAL) at Containerless Research, Inc. in Chicago, Illinois were performed. This technique allows for processing samples ranging in size from 2 - 3 mm and direct visual observation is possible. In prior experiments, samples were completely molten and solidified with either a cellular structure consisting of tetragonal $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$ coupled with fine dendrites of $\text{Y}_4\text{Ba}_3\text{O}_9$ or as single phase tetragonal $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$. These samples exhibited critical current densities on the order of 103 A cm^{-2} up to about 45 kOe

applied magnetic field at 5° K after a post-processing anneal in flowing oxygen. These experiments were extended to include processing of Gd and Nd substituted $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$ in collaboration with R.W. McCallum at Ames Laboratory. These rare-earth compounds are known to decrease the melting temperature of the material without adversely affecting the superconducting properties. In addition, a processing atmosphere of argon was used as well as dry air. Argon-processed samples exhibit large cracks and decompose to some of the more stable compounds in this system when exposed to air. The use of ultra high speed thermal imaging (UHSTI) for accurate temperature measurement over the entire sample surface proved successful, providing valuable solidification transition information.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 11/94 EXPIRATION: 11/96

PROJECT IDENTIFICATION: 962-25-08-22

NASA CONTRACT No.: NAG8-127

RESPONSIBLE CENTER: MSFC

Dimensional Stability of Supermatrix Semiconductors

PRINCIPAL INVESTIGATOR: Dr. Douglas E. Holmes

Electronic Materials Engineering

CO-INVESTIGATORS:

Weber, E.

Weber, Z.L.

Kendall, L.

University of California at Berkeley

Lawrence Livermore Laboratory

Electronic Materials Engineering

Task Objective:

Supermatrix Semiconductors (SMS) are composite semiconductor materials in which the phases form in oriented, periodic, and crystallographically aligned arrays. SMS technology makes possible the 3-dimensional superlattice and the extension of electronic and optoelectronic device technology to three dimensions. The objective of the program is to demonstrate microgravity as an enabling environment for producing SMS materials with a high degree of control over the morphology and dimensions of microstructural features as required for device fabrication. A broader understanding of growth-property relationships of multi-phase materials will also be developed.

Task Description:

Magnetically stabilized solidification is used to simulate microgravity conditions for the growth of SMS materials. Both Czochralski and Bridgman configurations are employed, and Ge/GeAs is the model SMS system. The impact of microgravity will be assessed by determining the dependence of microstructural features on magnetic field strength. Interface demarcation will provide a powerful research tool enabling the quantitative determination of macro- and microscopic interface shape and instantaneous interface solidification rate. Injection of time markers will also provide a means of studying the dynamics of morphological stability and microstructural adjustment to time and spatial fluctuations of solidification conditions. Microstructural and optoelectronic properties will also be characterized and correlated to growth conditions.

Task Significance:

Electronic Materials Engineering is a small business focused on establishing a new class of electronic materials called Supermatrix Semiconductors (SMS) for dual-use device applications. SMS's are multi-phase (composite) materials, and the phases form in oriented and periodic microstructures in 3 dimensions. Our motivation is to use SMS technology to extend existing electronic device technology, which is 2-dimensional, to 3 dimensions. An example is the quantum opto-electronic "Quantum Cable" for advanced optical data processing. High dimensional tolerance of the microstructural features will be required for device applications. Our early work in this field demonstrates the need for quiescent conditions unperturbed by convection in the melt to produce such SMS microstructures. The NASA program will demonstrate microgravity as an enabling environment for SMS production, and a broader understanding of basic growth-property relationships of multi-phase materials will be gained.

Progress During FY 1996:

The "Dimensional Stability of Supermatrix Semiconductors" contract was awarded to EME this year, and progress has been made in three areas since the program kick-off in June.

First, a presentation was made at the Microgravity Materials Science Conference (June 10-11, 1996, Huntsville, Alabama). The technical background of EME's unique project established prior to the NASA award was reviewed, and justification for microgravity research was presented and discussed. An excellent reception was received from conference attendees.

Second, the technical program was initiated. The first task involves the integration of existing Czochralski crystal growth equipment and a 9" electromagnet, which is expected to generate a field of up to about 8 kilogauss across the melt. This activity is ongoing, and task completion is anticipated in January 1997.

Third, the materials characterization task was begun. As an overall objective of the task is to compare the microstructure of SMS material produced with and without magnetic stabilization, baseline properties of crystals produced by the non-stabilized process will first be investigated. Ge/GeAs is the model system, and characterization is to initially concentrate on TEM and HREM.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-21-17

NASA CONTRACT NO.: NAS8-408

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Holmes, D.E. "Dimensional Stability of Supermatrix Semiconductors." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Non-Equilibrium Phase Transformations

PRINCIPAL INVESTIGATOR: Dr. Kenneth A. Jackson

University of Arizona

CO-INVESTIGATORS:

Zelinski, B.

University of Arizona

Task Objective:

Our computer simulations have resulted in a breakthrough in our fundamental understanding of phase changes which take place far from equilibrium. These phase changes are dominated by kinetics coupled to the thermodynamic properties of the material. The objective of this program is to explore the implications and insights provided by this breakthrough using computer simulations coupled with laboratory experimental studies.

Task Description:

The experiments involve an analysis of microsegregation that will ultimately require experimentation in a microgravity environment where the effects of convection are minimized. The program combines simulations with experimental studies, and both aspects are viewed as essential in that the simulations provide new insights for the experimental work, and the experiments verify important aspects of the simulations and keep them relevant to the real world. Experimental studies include the dopant segregation during the crystal growth of the semiconductor indium antimonide. Computer simulations predict the magnitude and orientation dependence of these effects. The simulations have been used to explore in detail the transition between two limiting regimes: 1) the diffusionless regime, where the interface must incorporate all the atoms as it moves, and 2) the rapid diffusion regime, where the atoms move rapidly compared to the rate of motion of the interface, and so dopant atoms can diffuse away ahead of an advancing interface, producing classical segregation effects. In the transition region between these two extremes the distribution coefficient (k -value) and the "kinetic phase diagram" depend on both the growth rate and the diffusion coefficient in the liquid, as well as on the orientation of the interface. The simulation results are in excellent agreement with experimental results on dopant incorporation into silicon. Simulations of other semiconductors as well as other materials systems, such as the crystallization of glasses, are being pursued.

Task Significance:

The structure and properties of materials produced by transformations that occur under conditions that are far from equilibrium is one of the central topics of materials science and is important for a variety of commercial processes including rapid solidification, spray powder formation, crystal growth, condensation processes, and glass formation. Non-equilibrium phenomena and segregation effects which are observed during rapid crystallization are not predicted by the standard quasi-equilibrium thermodynamic model. Our simulations capture, for the first time, the essence of these effects which occur in non-equilibrium transformations that occur in the real world. Our Monte Carlo computer simulations predict that these phenomena depend on the undercooling, on the growth rate, and on the diffusion coefficient in the fluid phase. These effects are generally important in the regime where the phase transformation takes place far from equilibrium. Projects supported by NASA using levitation and the microgravity environment are making major contributions to our understanding of nucleation and crystallization under these conditions, in the regime where these non-equilibrium effects are very important. Our simulation results provide a new framework for the interpretation of these experiments.

Progress During FY 1996:

The analytical model which describes the orientation dependence, the growth rate dependence and the composition dependence of the segregation coefficient has been further developed and its predictions have been compared with experimental results. Using Monte Carlo computer simulations, the orientation dependence of the segregation coefficient (k -value) has been determined for several different growth directions. It has been determined that, in the simulations, the orientation effects come from the difference in step density and step velocity for the different crystallographic faces. The step density can be determined in the simulations, and it is found that the orientation dependence of the k -value is given by the growth rate squared divided by the step density on the growth face. The simulation results are in excellent agreement with experimental measurements of the orientation dependence of the k -value for Bi incorporation into Si. Simulations have also been carried out for growth on Si (100) at small undercoolings, where the growth rate is controlled by nucleation. The growth rate from the simulations has been

fitted using conventional nucleation theory. The Bridgman apparatus constructed for the growth of crystals of indium antimonide has been used to grow doped crystals, and the dopant distribution has been measured. The effect of convection on the dopant distribution depends of the degree of care which is taken during all phases of the growth process. The apparatus includes Peltier pulsing to determine the growth rate, and the actual growth rate has been found to be significantly different from the nominal growth rate. The singularity in the growth rate observed in ammonium chloride - water dendrites has been shown to be of different origin than the singularity observed in metal alloy dendrites.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 2/93 EXPIRATION: 2/96

PROJECT IDENTIFICATION: 962-25-08-29

NASA CONTRACT NO.: NAG8-123

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Jackson, K.A., Gilmer, G.H., and Temkin, D.E. Monte Carlo Simulation of the Rapid Crystallization of Bismuth-doped Silicon. Phys. Rev. Letters, vol. 75, 2530 (1995).

Jackson, K.A., Gilmer, G.H., Temkin, D.E., and Beatty, K.M. Microsegregation Far From Equilibrium. J. Cryst. Growth, vol. 163, 461 (1996).

Presentations

Beatty, K.M., and Jackson, K.A. "Orientation Dependence of the Distribution Coefficient (k-value) Obtained from a Spin-1 Ising Model." Tenth American Conference on Crystal Growth, Vail, Colorado, August 6, 1996.

Blackmore, K., Beatty, K.M., Hui, M., and Jackson, K.A. "Growth Behavior of $\text{NH}_4\text{Cl-H}_2\text{O}$ Mixtures." Tenth American Conference on Crystal Growth, Vail, Colorado, August 8, 1996.

Hui, M., Beatty, K., Blackmore, K., and Jackson, K.A. "Impurity Distribution in InSb Single Crystals." Tenth American Conference on Crystal Growth, Vail, Colorado, August 6, 1996.

Jackson, K.A. "Monte Carlo Simulation Of Non-equilibrium Segregation During Crystal Growth." Cornell University, November 14, 1995.

Jackson, K.A. "Non-equilibrium Segregation During Crystallization." Microgravity Materials Science Conference, Huntsville, June 10-11, 1996.

Jackson, K.A. "Non-equilibrium Segregation During Crystallization." Conference on Structural and Dynamic Modeling of Mechanical Behavior of Solids, Monte Verita, Switzerland, September 5, 1996.

Dislocation Formation during Growth of Semiconductor Crystals

PRINCIPAL INVESTIGATOR: Dr. Monica L. Kaforey

Case Western Reserve University

CO-INVESTIGATORS:

Matthiesen, D.
Chait, A.Case Western Reserve University (CWRU)
NASA Lewis Research Center (LeRC)

Task Objective:

The objective of this research is to study the effect of free surface formation on the dislocation density of directionally solidified doped semiconductor crystals and to correlate these results with appropriate numerical modeling efforts. The proposed sample material is germanium doped to $10^{18}/\text{cm}^3$ gallium.

Task Description:

During directional solidification of semiconductor crystals, dislocations propagate from the existing seed crystal into the growing crystal at the melt/solid interface and from the solid/crucible surface into the growing crystal. This proposed work will investigate the effect of forced contact versus detachment of the melt from the crucible wall on dislocation structure during directional solidification of semiconductor crystals.

Ground-based research will include verifying the sample-ampoule design and its interaction with the furnace. The characterization methods to be used on the samples will be developed, including a technique for determining the dislocation density in the samples. Numerical simulations will be compared to the experimental results.

Task Significance:

In the ongoing efforts to produce higher quality semiconductor materials, there is a continuous search for ways to consistently make materials with fewer defects. Dislocations are the specific type of defects being examined in this investigation. The knowledge gained from these experiments, combined with a vigorous modeling effort, is expected to contribute significantly to the understanding of how and why dislocations form during the growth of semiconductors. This information will be useful to ground-based research efforts that are trying to reduce the number of defects in semiconductor crystals and could lead to the production of better materials.

Progress During FY 1996:

Funding for this project began late in the fiscal year. During the short reporting period, refurbishing and updating of equipment was started.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/96 EXPIRATION: 6/98

PROJECT IDENTIFICATION: 962-21-18

NASA CONTRACT NO.: NAG8-126

RESPONSIBLE CENTER: MSFC

The Role of Dynamic Nucleation at Moving Boundaries in Phase and Microstructure Selection

PRINCIPAL INVESTIGATOR: Dr. Alain S. Karma

Northeastern University

CO-INVESTIGATORS:

Trivedi, R.

Iowa State University

Task Objective:

Nucleation at moving boundaries and the growth competition between different phases play crucial roles in the selection of phases and solidification microstructures. Some important examples include the formation of layered structures in peritectic systems, the formation of metastable phases in highly undercooled droplets, and the selection of phases and microstructures in strip cast stainless steels. The complexity of accurate theoretical modeling, and the difficulty of precise critical experimental study, have prevented a fundamental understanding of this important class of microstructure selection problems.

So far, the prediction of phase and microstructure selection has been based on heterogeneous nucleation on a static interface and/or comparing the relative growth rate of different phase/microstructures (i.e., planar, cellular, dendritic, or eutectic) under steady-state growth conditions. The formation of new phases, however, occurs via nucleation on a moving boundary. The actual phase and microstructure selection is controlled by complex interactions between the nucleation process and the growth competition between the nuclei and the preexisting phase under non-steady-state conditions.

This research addresses the critical role of nucleation at moving boundaries in the selection of phases and solidification microstructures through experiments in peritectic and eutectic systems and the development of reliable numerical models.

Task Description:

The proposed research will consist of carrying out accurate and rigorous numerical modeling, coupled with critical ground-based and microgravity experimental studies, to quantitatively evaluate the process of nucleation on a moving boundary and the dynamical selection of phases and microstructures.

In phase I of this study, we shall concentrate on the nucleation occurring in peritectic systems where, for a specific range of compositions in the two-phase region, a layered structure is observed in which two phases alternate perpendicular to the growth direction. The spacing, morphology, and composition variations of these nearly planar layers are dictated by the nucleation at the moving boundary and by the relative growth rates of the nuclei and the preexisting phase. Directional solidification of peritectics gives a unique opportunity to examine this nucleation under well controlled experimental conditions.

In phase II, we shall model and examine through directional solidification the problem of nucleation at moving boundaries in the selection of phases with different microstructures in peritectic and eutectic systems. Growth conditions will be studied that give rise, in peritectics, to alternate layers of cellular and planar front microstructures, and, in eutectic systems, to alternate layers of eutectic and planar front microstructures.

In phase III, experiments under microgravity conditions will be performed to investigate layer formation in bulk samples in the absence of convection. Ground-based experiments have already shown that, at low velocity, convection effects can destabilize the formation of the layers and suppress the nucleation of the new phase.

Task Significance:

The ability to predict the microstructure that gives the desired properties to a material is a key ingredient for successful solidification processing and for the control of cast products. Basic concepts of nucleation at moving boundaries and phase and microstructure selection obtained through this study will provide a fundamental theoretical basis to model reliably important advanced materials such as magnetic, rare earth, and high temperature superconductors found in peritectic systems.

Progress During FY 1996:

The formation of banded microstructure in peritectic systems was examined theoretically as well as experimentally in a convective regime. A model was developed that describes the non-steady-state growth of alternate solid a and b phase bands with a planar solid-liquid interface and incorporates the effect of convection by assuming that solute diffusion takes place within a boundary-layer of constant thickness, with a uniform composition in the mixed liquid zone outside this layer. The model predicts that convection destabilizes banding in such a way that only a few bands with a variable width are formed in a finite sample, and that this transient banding process can occur over almost the entire range of composition inside the two-phase peritectic region. Ground-based directional solidification studies in the Pb-Bi system were carried out to test the model predictions. The experimental results were found to reproduce the basic features of the banded structures that are predicted by the model for a convective system. However, the basic mechanism of band formation in the Pb-Bi system was found to be significantly different from the nucleation at the boundary of the pre-existing phase, and two new mechanisms for the formation of bands were identified and described.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-21-38

NASA CONTRACT NO.: NAG8-125

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Karma, A., and Trivedi, R. "Role of Dynamics Nucleation at Moving Boundaries in Phase and Microstructure Selection."
NASA Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.

Identification of Gravity-Related Effects on Crystal Growth from Melts with an Immiscibility Gap

PRINCIPAL INVESTIGATOR: Dr. Mohammad Kassemi

Ohio AeroSpace Institute

CO-INVESTIGATORS:

Chait, A.

Sayir, A.

Farmer, S.C.

NASA Lewis Research Center (LeRC)

Case Western Reserve University (CWRU)

NASA Lewis Research Center (LeRC)

Task Objective:

This work encompasses a detailed experimental-numerical approach to study the effects of natural and Marangoni convections on solidification of single crystals from a silicate melt with a liquid-liquid immiscibility gap. The main objective of this work is to determine the necessary conditions for growing superior quality single crystals from the phase separated melt by isolating the effects of convection and the other interacting transport processes.

Task Description:

Very little work has been done or published with regard to solidification from immiscible liquids. In this work, we use a combined experimental-numerical approach to study the role of gravity-driven convection on growth of single crystal mullites from the melt. High resolution digital images obtained in our laboratories at NASA Lewis demonstrate that mullite formation is preceded by a state of liquid-liquid immiscibility. To our knowledge, this is the first direct experimental evidence of liquid immiscibility reported for this system. Preliminary experimental results also reveal that mixing in the melt caused by density-driven convection can significantly affect the immiscibility of the liquid and result in different crystalline forms (stable or metastable crystalline phases; polycrystals or single crystals). The transport processes affecting concentration and temperature gradients in the melt and in the growing solid are quite complicated for silicate systems. The immiscibility of the liquid, segregation of dopant, and interface shape are not only directly affected by density-driven and Marangoni convection in the melt but are also indirectly influenced by a significant amount of radiation and conduction heat transfer through the semi-transparent solid. The interaction between the various transport processes are further complicated by the observed multi-layered fluid structure.

During the course of this investigation, the effect of density-driven convection on the liquid-liquid immiscibility will be experimentally investigated in a series of controlled ground-based tests by growing crystals over a wide range of diameters (from 100 microns to 2 cm). This allows us to vary the intensity of natural convection by several orders of magnitude. The effect of surface tension forces will be studied by varying the Al/Si concentration of the materials and through dopant additions. The impact of thermal radiation on the liquid-solid interface shape and on the degree of homogenization in the melt will be studied by changing the dopant concentration (at fixed Al/Si compositions) which directly alters the transparency of the material. A comprehensive numerical model will be developed by formulating the simultaneous effects of natural and thermocapillary convection, moving boundaries, and semi-transparent radiation heat transfer. The numerical model will be used in conjunction with the test results to isolate the interacting phenomena. Finally, the type and quality of crystal produced (void formation, ordering, dislocation density, and low angle grain boundaries) will be characterized using scanning electron, transmission electron, and atomic force microscopy. The crystal characteristics will be correlated to the growth conditions and their effect on the transport.

Task Significance:

Industrial use of crystals grown from silicate melts is becoming increasingly important in electronic, optical, and high temperature structural applications. Even the simplest silicate systems like $\text{Al}_2\text{O}_3\text{-SiO}_2$ have had, and will continue to have, a significant role in the development of traditional and advanced ceramics. A unique feature of crystals grown from the silicate systems is their outstanding linear electro-optic properties. They also exhibit exceptionally high optical rotativity. As a result, these crystals are attractive materials for dielectric, optical, and microwave applications. Preliminary experimental work in our laboratory has indicated that directional solidification of a single crystal mullite appears to be preceded by melt segregation where a liquid slightly enriched in Al_2O_3 is encapsulated in a SiO_2 -rich liquid. Disruption of the segregated state results in crystallization of a two

phase structure. There is also evidence that mixing in the melt caused by density-driven convection can significantly affect the immiscibility of the liquid and result in different crystalline forms (stable or metastable crystalline phases; polycrystals or single crystals). On earth, the immiscible state has only been observed for small diameter crystals grown in float zone systems where natural convection is almost negligible. Therefore, it is anticipated that growth of large single crystals from silicate melts using the Bridgman technique as proposed here would benefit from the microgravity conditions because of the reduction of the natural convective mixing.

Progress During FY 1996:

Since the grant only started in September 1996, we have no progress to report as of this writing.

STUDENTS FUNDED UNDER RESEARCH:**TASK INITIATION: 5/96 EXPIRATION: 5/97****PROJECT IDENTIFICATION: 962-21-29****NASA CONTRACT NO.: NAG8-86****RESPONSIBLE CENTER: MSFC**

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Kassemi, M., Sayir, A., Farmer, S., and Chait, A. "Identification of Gravity-Related Effects on Crystal Growth from Melts with an Immiscibility Gap." The Third Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.

Combined Heat Transfer Analysis of Crystal Growth

PRINCIPAL INVESTIGATOR: Dr. Mohammad Kassemi

Ohio Aerospace Institute

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The technical objective of this proposal is to provide a quantitative understanding of the effects of radiation heat transfer on crystal growth in low-gravity space experiments. To accomplish this goal a generalized combined conductive-convective-radiative numerical model is developed which can accommodate various crystal growth experiments.

Task Description:

Radiation heat transfer affects crystal growth in both space and ground-based processing. This is due to the high operating temperatures of the crystal growth processes, the semitransparency of the crucible and phase change materials and the heat transfer link between the crucible and the furnace. In ground based experiments, radiation and convection coexist and compete for controlling the heat transfer process. However, the role of radiation heat transfer is more prominent in low-gravity environment of space where convection heat transfer is minimized. A numerical methodology was developed for radiation heat transfer in the generalized multi-dimensional cylindrical geometries encountered in crystal growth. The radiation scheme which is based on the Discretized Exchange Factor method (DEF) uses node-to node exchange to calculate radiation heat transfer in a generally absorbing, emitting, scattering media. The main advantage of the DEF method is its accuracy. Another advantage of the present approach is that the radiation model can be easily incorporated into existing finite difference and/or finite element formulations. The radiation model was incorporated into a finite element code for fluid flow and heat transfer and a generalized combined conduction, convection, radiation model was developed for crystal growth in cylindrical ampoules. The radiation model takes into account the wavelength-dependant semitransparency of crystals such as BSO. The solution algorithm tracks the movement of the interface during the solidification process and adjusts the finite element mesh to accommodate changes in the shape and position of the growing solid. Radiation view factors are continuously updated as the geometry is altered. The model is applied to existing experiments and used to demonstrate the role of radiation under low gravity environment.

Task Significance:

Thermal radiation governs the energy balance in many Earth and space processes. It plays a crucial role in the production of glasses, semi-conductors, and advanced pay-off materials such as optical crystals. Low-gravity simulations performed using the combined heat transfer model, clearly indicate that radiation effects are dominant during low gravity solidification of oxide crystals, such as BSO. Nonuniform radiation loss from the solidification front can cause highly stretched and curved interfaces during low gravity experiments in ways that may deteriorate the quality of the growing solid. Consequently, the numerical models that do not rigorously include radiation effects cannot be used to predict the correct shape and movement of the solidification front.

Progress During FY 1996:

The early studies undertaken during the course of this research dealt with growth of pure oxide crystals such as BSO and YAG. In their pure form these materials are fully transparent to radiation below 6 microns. At operating temperatures associated with solidification of BSO and YAG more than 85% of emission is within these transparent bands. Therefore, pure oxide crystals are subject to radiation loss through the solid which acts like a heat pipe. Addition of even small amounts of dopant can change the radiative characteristics of the solid by increasing its absorption capability. In this case, volumetric radiation absorption and emission in the solid become important. This has been the main focus of the work in FY95 and FY96.

A new banded nongray radiation model was developed to compute volumetric radiation exchange during crystal growth. The radiation model considers a generalized absorbing emitting scattering nongray media. The methodology is based on a variation of DEF method which evaluates radiative transfer between any two points within the domain using node-to node exchange. The volumetric radiation model was tested against other well established methods for

computing radiation such as YIX, Finite Volume, Discrete Ordinate, and P3 Differential Approximation and also experimental results based on benchmark cases. The comparisons indicate excellent agreement with experimental results and prove that the new methodology has better accuracy compared to the other commonly used techniques. The volumetric radiation model was encoded and incorporated into the finite element code Fidap. The code was then customized to investigate solidification of YAG, BSO, and Sapphire.

The radiation model was used to simulate the volumetric radiative cooling which dominates growth of Sapphire fiber crystals from melt. The numerical predictions compared well with the experimental results provided by A. Sayir (Case Western Reserve University) and the analytical solutions derived by S. Korpela (Ohio State University).

Solidification of BSO and YAG were also investigated for both low-gravity and ground-based experiments. The effect of an increase in absorption coefficient which can be brought about by addition of dopants was examined for various microgravity and ground-based applications. The numerical results indicate that for BSO and YAG an increase in the absorption and emission in the solid reduces radiation loss from the interface during the growth process. Consequently, as the opacity of the solid increases, the extent of the interface curvature and stretching decreases. This also results in weakening of the recirculating vortices next to the interface in the melt. The results show that for both low-g and 1-g solidification experiments of semitransparent oxides, increased absorption in the solid caused by addition of small amounts of dopants can have profound effects on the interfacial heat balance, cooling rate in the solid, shape of the crystal and flow structures in the melt.

The numerical simulations proved to be extremely costly and CPU-intensive. This is mainly due to the necessity of calculating radiation view factors every time the shape of the crystal changes during the simulation of the solidification process. Therefore, two approaches are being pursued in order to reduce simulation times:

1. *different computational grids for the convection and radiation calculations.* Since radiative heat transfer is more forgiving as far as grid density requirements are concerned, larger elements can be considered for radiation calculations which reduce the number of view factor calculations drastically.

2. *The Discrete Ordinate method.* The Discrete Ordinate method does not require view factor calculations. Therefore, it is computationally more efficient than the DEF method. Unfortunately, there is a loss in accuracy which has to be properly assessed.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 1/93 EXPIRATION: 1/96

PROJECT IDENTIFICATION: 962-21-05-10

NASA CONTRACT No.: NCC3-411

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Korpela, S., Chait, A., and Kassemi, M., Radiative heat transfer in fiber drawing and crystal pulling. Journal of Crystal Growth, (1996).

Proceedings

Kassemi, M., and Naraghi, M.N.H., "Interaction of radiation with conduction and convection in solidification of oxide crystals." Proceedings of the International Symposium on Radiative Heat Transfer, International Center for Heat and Mass Transfer, Begell House Inc., New York, 1996.

Presentations

Kassemi, M., and Naraghi, M.N.H., "Application of discrete exchange factor method to combined heat transfer problems in cylindrical media." International Mechanical Engineering Congress and Exposition, November 1996.

Measurement of Liquid-to-Solid Nucleation Rates in Undercooled Metallic Melts

PRINCIPAL INVESTIGATOR: Dr. Joseph L. Katz

Johns Hopkins University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The main objective of this research is to obtain quantitative experimental measurements of liquid-to-crystal homogeneous nucleation rates in a variety of undercooled metallic melts. The proposed apparatus will allow these measurements to be made in 1-g. However, a version optimized to take advantage of microgravity would enable one to extend the range of melt compositions and droplet sizes. Thus a second objective of this work is to establish the foundation needed for the design, construction, and use of a future space-based apparatus.

Task Description:

A novel combination of proven techniques is being used. Pure droplets will be formed in ultrahigh vacuum using electrohydrodynamic atomization to produce diameters in the range 5 to 10 microns. Since the atomizer feedstock is melted only at its tip, there is no possibility of contamination (except from residual vacuum chamber gases, which will introduce negligible contamination because the duration of the experiments will be limited). Because of their very small size, most of the droplets will be free of nucleation catalysts.

A single charged droplet will be captured from the electrohydrodynamic atomization spray in an electrodynamic particle trap operating in the same ultrahigh vacuum system and positioned opposite the atomizer. Droplet size will be determined by measuring angular light scattering intensities. The droplet will freeze at some point to form a solid particle. A visible light laser will provide the heat to melt the particle and control its temperature. The particle's temperature will be measured by its emissive power using single-color pyrometry. To determine the time-temperature dependence of the rate of crystal nucleation, ensembles of time-temperature profiles will be generated by repeated undercooling experiments on single samples. Statistical fluctuations in the time at which nucleation occurs will be analyzed to determine the time and temperature dependence of the nucleation frequency. The planned experimental approach will allow us to melt, cool, and solidify metallic droplets free from both particulate and surface nucleation catalysts. At no time, from formation of the droplets until the end of the experiment, will the droplet be in contact with any foreign surface, or fluxing agent. Furthermore, the droplet will never be exposed to gases of any composition for a period of time long enough to affect its surface (except those we deliberately add).

We plan to begin by making quantitative measurements of the rate of homogeneous liquid-to-crystal nucleation in a variety of pure metallic melts, starting with gold, lanthanum, neodymium, praseodymium, uranium, and germanium (a semi-metal). The first results to be obtained are experimental data on homogeneous nucleation rates in undercooled single-component metallic melts as a function of their temperature-time history. This study then will be expanded to alloys, including glass-forming alloys. Studies which take advantage of the planned apparatus' capability to expose samples to known concentrations of gaseous reactants are also planned.

Task Significance:

The solidification of deeply undercooled metals has led to the production of many new and valuable materials. The limit to such undercooling is set by the nucleation of crystallites within the material. However, despite the ubiquity of liquid-to-crystal nucleation phenomena, both in nature and in commercial materials processes, they are still poorly understood and are not very reproducible. Past experimental studies have faced persistent difficulties because crystal nuclei production is strongly catalyzed by contact with foreign particles and with external surfaces. Furthermore, it has proven difficult to obtain contactless temperature measurements precise enough to probe the very strong dependence of the nucleation rate on temperature. These difficulties will be circumvented by these experiments. These results will also be of great importance to NASA's goal of enabling containerless processing techniques.

Progress During FY 1996:

The Molten Metal Droplet Levitator design was finalized and is being constructed.

STUDENTS FUNDED UNDER RESEARCH:**TASK INITIATION:** 4/96 **EXPIRATION:** 4/00**PROJECT IDENTIFICATION:** 962-21-39**NASA CONTRACT No.:** NAG8-125**RESPONSIBLE CENTER:** MSFC

Fundamentals of Thermomigration of Liquid Zones Through Solids

PRINCIPAL INVESTIGATOR: Prof. Michael J. Kaufman

University of Florida

CO-INVESTIGATORS:

Abbaschian, R.

University of Florida

Gokhale, A.

University of Florida

Task Objective:

Currently, significant resources in terms of expert manpower as well as direct costs are being expended to develop advanced materials such as the high-temperature structural intermetallics MoSi_2 and NiAl , and the fast semiconductors GaAs and GaSb . Despite considerable efforts in these areas, the intrinsic properties of many of these compounds, and alloys based on them, remain poorly understood to the degree needed to enhance their development and application. For example, it is unclear if the brittle nature of many of the intermetallics of current interest is an intrinsic property of these compounds or is associated with interstitial impurities or impurity phases. Consequently, there is a need not only to produce single crystals of controlled purity, perfection and orientation, but also to understand the details of interfacial atomistics during crystal growth in order to bring about such control.

For many of the exotic compounds of technological interest currently, conventional crystal growth techniques have not proven successful in this regard because of the many problems associated with container contamination or loss of stoichiometry due to preferential vaporization of one or more of the elements with high vapor pressures (e.g., arsenic in GaAs , antimony in GaSb , silicon in MoSi_2 , and aluminum in NiAl). In addition, these conventional techniques are not amenable to a scientific study of correlations between thermosolutal convection and key aspects of crystal growth such as the interface (growth) temperature and morphological stability. For example, the use of electromagnetic induction to produce float zones introduces an additional electromagnetic stirring component in the liquid zone and also precludes the use of most sensors to measure interface temperatures.

Task Description:

Although this method was discovered more than 35 years ago, there have been few attempts to utilize it as a means for processing materials in spite of the fact that most materials typically can be processed (e.g., grown as single crystals, joined and sectioned) at temperatures well below their melting points. In addition, coupling of this scheme with both acoustic emission/reflection and possibly Seebeck techniques should allow the interface positions, zone length, and interface temperature to be monitored *in situ* in real time.

Task Significance:

The focus of this research is intended to circumvent the common problems (e.g., crucible contamination and loss of stoichiometry) associated with conventional crystal growth methods by using the relatively unique technique of TGZM to grow single crystals of materials of current technological interest. In addition, the low-growth temperatures require much lower power inputs and result in enhanced safety during both ground operations and spaceflight. Also, it is anticipated that significant, hitherto unavailable data on liquid diffusivities will be generated during these experiments. Finally, it should be emphasized that the capability of producing high quality, inexpensive crystals of some of these rather exotic compounds could greatly facilitate advancements in these fields of current technological interest.

Progress During FY 1996:

Research efforts in FY96 concentrated on characterization of thermomigration of liquid aluminum zones through $\langle 100 \rangle$ and $\langle 111 \rangle$ single crystal silicon wafers subjected to stationary temperature gradients. In addition, attempts were made to determine the rate controlling step for thermomigration: either diffusion across the molten solvent zone or dissolution/deposition at the solid-liquid interfaces. Thermomigration of the molten aluminum zone through $\langle 111 \rangle$ silicon wafers produced continuous zones with planar solid-liquid interfaces. $\langle 100 \rangle$ type wafers, however, showed rather discontinuous zones with irregular, triangle-shaped zone segments. Determination of the rate controlling step was based on establishing a relationship between migration rate and zone thickness. Results from this portion of the study proved inconclusive resulting most likely from non-uniform wetting as a result of

oxidation. Continuing work on this system is focused on overcoming the oxidation at the solid-liquid interface and also on attempts at assessing the three dimensional nature and characteristics of a planar zone propagating through single crystal silicon wafers.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	1
PhD Students:	1	PhD Degrees:	0

TASK INITIATION: 2/93 **EXPIRATION:** 2/96**PROJECT IDENTIFICATION:** 962-21-08-16**NASA CONTRACT NO.:** NAG8-946**RESPONSIBLE CENTER:** MSFC

Compositional Dependence of Phase Formation and Stability

PRINCIPAL INVESTIGATOR: Dr. Kenneth F. Kelton

Washington University, St. Louis

CO-INVESTIGATORS:

Robinson, M.

NASA Marshall Space Flight Center (MSFC)

Rath, T.

NASA Marshall Space Flight Center (MSFC)

Task Objective:

The objectives of this research are to extend computer models developed by us to model first order phase transformations involving cases where the composition of the final phases are different from those of the initial ones. This study is important to resolve conflicts in the experimental literature, to develop theoretical methods for treating both steady state and time dependent nucleation in a partitioning system, to extend the understanding of basic nucleation phenomenon, and to aid in the eventual development of techniques for making qualitative predictions of desired phases and microstructures. This research will lead to improved methods for analyzing thermoanalytic data that will have wide applicability for phase transformations studies. In particular, it will aid in the design and data analysis of remote experiments, such as might take place in a microgravity environment. Drop-tube experiments may reveal new effects of composition on the nucleation of related complex periodic and quasiperiodic phases that will likely suggest future containerless solidification and microgravity studies.

Task Description:

The steady state and time-dependent nucleation rates as a function of temperature and SiO_2 concentration will be measured in one pseudo-binary silicate glass, $\text{Na}_2\text{O} \cdot \text{CaO} \cdot 3\text{SiO}_2$. Initial work by others suggests a strong compositional dependence of the steady state nucleation rate, though the dependence of the transient behavior has not been measured. The concentration dependence of the maximum undercooling in drop-tube experiments in Ti-Mn-Si and Al-Cu-Co-Si, and if time permits, Ti-Cr-Si and Ti-Ni-Zr-Si, all metallic liquids that form quasicrystals, will be measured. These data will be used to refine a model, developed previously by us, of the magnitude and time dependence of the nucleation rate as a function of composition. That model for nucleation will then be incorporated in our numerical model for phase transformations. Initial tests of that extended model will be made by comparing calculated and measured trends of DSC data for the devitrification of $\text{Na}_2\text{O} \cdot \text{CaO} \cdot 3\text{SiO}_2$ glass as a function of SiO_2 concentration.

Task Significance:

Although in most situations solid phases grow from liquids having a different composition, systematic work focusing on the development of the correct treatment of phase nucleation under these conditions is needed. We are therefore carrying out a theoretical and experimental investigation of the nucleation and crystallization kinetics in model silicate and metallic systems. The insight and new theoretical framework gained from this work will enhance our basic understanding of nucleation, provide new insights into solidification processes and lead to new methods, based on computer simulations, that will allow the analysis of crystallization data under isothermal and nonisothermal conditions. One specific application of these new methods will be the analysis of data obtained remotely, such as in a microgravity environment. This work will ultimately enhance our ability to predict and control microstructural development, which is essential to the development of new materials to meet changing technological needs.

Progress During FY 1996:

During the past year, experimental and theoretical investigations of the compositional dependence of the nucleation rate and transient time were conducted.

1. The ability to levitate and melt Ti-3d transition metal-Si-O samples of the desired composition was demonstrated. To better collect undercooling data by improving the position stability of the melted alloys within the rf coil, smaller samples of Ti-Cr-Si and Ti-Cr-Si-O and new samples Ti-Mn-Si-O and Ti-Ni-Zr, which also form phases with local icosahedral order, were prepared.

2. We have completed a comparison between experimental data of the time-dependent nucleation rates in $\text{Na}_2\text{O} \cdot \text{CaO} \cdot 3\text{SiO}_2$ as a function of SiO_2 concentration and computer predictions based on a quantitative model of cluster evolution. These studies suggest that the observed changes are best described by a composition dependence of the interfacial free energy between the glass and the stoichiometric crystal phase.

3. To accurately model time-dependent nucleation processes governed by the diffusive flux in the initial phase, we have developed a theory of diffusion limited nucleation which couples the stochastic nature of cluster evolution with the evolving diffusion fields near the cluster. The resulting differential equations are much more stiff than the set of coupled equations central to the classical theory. They have been solved only in the limits of small times.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/94 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-26-08-14

NASA CONTRACT No.: NCC8-85

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Kelton, K.F., Lakshmi Narayan, K., Levine, L.E., Cull, T.C., and Ray, C.S. Computer Modeling of Nonisothermal Crystallization. *J. Non-Cryst. Solids*, (1996 in press).

Lakshmi Narayan, K., Kelton, K.F., and Ray, C.S. Effect of Pt Doping on Nucleation and Crystallization in $\text{Li}_2\text{O} \cdot 2\text{SiO}_2$ Glass: Experimental Measurements and Computer Modeling. *J. Non-Cryst. Solids*, vol. 195, 148-157 (1996).

Levine, L.E., Narayan, K.L., and Kelton, K.F. Finite size corrections for the Johnson-Mehl-Avrami-Kolmogorov Equation. *J. Mater. Res.*, (1996 in press).

Ray, C.S., Day, D.E., Huang, W., Lakshmi Narayan, K., Cull, T.S., and Kelton, K.F. Nonisothermal Calorimetric Studies of the Crystallization of Lithium Disilicate Glass. *J. Non-Cryst. Solids*, (1996 in press).

Proceedings

Kelton, K.F. "Kinetic Analysis of Nonisothermal Crystallization (Invited Talk)." Proceedings of the Materials Research Society (MRS), Thermodynamics and Kinetics of Phase Transformations (J.S. Im, B. Park, A.L. Greer, and G.B. Stephenson, eds), vol. 398 (1995).

Presentations

Lakshmi Narayan, K., and Kelton, K.F. "Composition Effects on Nucleation and Growth in $\text{Na}_2\text{O} \cdot 2\text{CaO} \cdot 3\text{SiO}_2$ glasses." Mid-West Solid State Conference, St. Louis, Missouri, October 1996.

Phase Formation and Stability: Composition and Sample-Size Effects

PRINCIPAL INVESTIGATOR: Dr. Kenneth F. Kelton

Washington University, St. Louis

CO-INVESTIGATORS:

Robinson, M.

NASA Marshall Space Flight Center (MSFC)

Rath, T.

NASA Marshall Space Flight Center (MSFC)

Task Objective:

The objectives of this research are the examination of the consequences of solute partitioning on nucleation and growth processes. Though diffusion-limited growth has been well studied, only limited investigations of the effects of partitioning on the nucleation rate of the new phase exist. Key studies carried out in this research will result in the development of a model for nucleation that is appropriate for the more common crystallization case, where the compositions of the initial and final phases differ (primary crystallization). This will allow computer models already developed and tested by us for phase transformations involving no compositional change to be extended to include primary crystallization. The insight gained and the models developed in these studies will lead to improved methods of analysis for thermoanalytic data that will have a wide applicability for phase transformation studies. In particular, this will make calorimetric experiments, which are easily performed in remote locations, of use for materials studies in a microgravity environment. Drop-tube experiments on liquids that transform by primary crystallization to complicated crystal and quasicrystal structures will lead to new space shuttle and space station microgravity studies.

Task Description:

Steady-state and time-dependent nucleation rates will be measured in select silicate and metallic glasses and liquids. Growth rates and driving free energies, determined as a function of composition, will be used to analyze these data. The concentration dependence of the maximum undercooling for Ti-Cr-Si, Ti-Cr-Si-O and Ti-Zr-Ni, liquids that form quasicrystals and complex crystalline phases, will be studied using the drop-tube facility at Marshall Space Flight Center to further investigate shifts in interfacial free energy with composition. Crystallization of silicate glasses and the new, strongly metastable, metallic glasses will be studied to determine the effects of partitioning on the nucleation. We will develop a new model that takes into account compositional effects on both the kinetic and thermodynamic aspects of time-dependent nucleation. Our experimental data will be used to test and to refine that theory. This new model for nucleation will be incorporated into our numerical calculations of phase transformations, which will be tested by predictions with measured trends of differential scanning calorimeter studies of devitrification in the silicate and metallic glasses studied.

Task Significance:

Although crystallization of liquids and glasses generally results in phases having a different composition from that of the initial liquid or glass (primary crystallization), the understanding of nucleation and growth in such cases is unclear. This lack of knowledge makes the quantitative analysis of crystallization kinetic data impossible and hinders the predictive design of modern materials. Our combined experimental and theoretical studies of the crystallization of silicate and metallic glasses and liquids as a function of composition, will elucidate the role of thermodynamic and kinetic parameters on the nucleation and growth behavior and will guide the development of a new theory of nucleation. When coupled with existing theories of growth, this new model for nucleation will enable a numerical model developed previously by us for constant composition phase transformations to be extended to this more common case. The insight and new theoretical framework established by this research will enhance our understanding of nucleation and growth processes and will lead to new methods for the analysis of crystallization kinetic data, which will have wide applicability. Since these data are easily obtained in a remote environment, when properly analyzed they can provide a powerful probe for materials studies in a microgravity environment. Finally, the understanding gained from this study is crucial for extending well established methods of phase prediction and microstructural control to the more common cases of primary crystallization.

Progress During FY 1996:

Since the initiation of this grant in Spring, 1996, initial surveys have been made to determine the appropriate systems for the studies of the compositional dependence of time-dependent nucleation and some experimental and theoretical investigations have commenced.

1. Experimental studies of the effect of pre-annealing treatments on the time dependent nucleation behavior in $\text{Na}_2\text{O} \cdot \text{CaO} \cdot 3\text{SiO}_2$ as a function of SiO_2 concentration have begun. Initial results from the stoichiometric glass are in agreement with predictions based on a quantitative model of cluster evolution in polymorphic systems. Similar comparisons as a function of composition will provide a probe into the cluster dynamics that will better determine whether the nucleation behavior is indeed governed by a changing interfacial energy with composition or whether coupling of the diffusive and cluster interfacial fluxes is significant.
2. Undercooled samples of $\text{Ti}_{60}\text{Cr}_{30}\text{Si}_{10}$, $\text{Ti}_{61}\text{Mn}_{33}\text{Si}_6$, $\text{Ti}_{61}\text{Mn}_{37}(\text{SiO}_2)_3$, and $\text{Ti}_{61}\text{Mn}_{37}\text{Si}_2(\text{SiO}_2)_4$ have been processed in the NASA 100 m drop tube, located at the Marshall Space Flight Center. Techniques have been developed for preparing these samples for transmission electron microscopy investigations. Initial TEM studies of the phase microstructure have begun.
3. Several Ti-based and Zr-based metallic glasses have been prepared and initial investigations have been made of their crystallization properties. These glasses were chosen to have sluggish crystallization kinetics so that nucleation measurements following multiple-step annealing treatments (of the kind already underway in the silicate glasses) might be possible. The $\text{Zr}_{65}\text{Cu}_{17.5}\text{Ni}_{10}\text{Al}_{7.5}$ and $\text{Zr}_{69.5}\text{Cu}_{12}\text{Ni}_{11}\text{Al}_{7.5}$ glasses, which devitrify by primary crystallization to a phase mixture containing quasicrystals, appear most promising for the nucleation studies proposed.
4. A theory of diffusion limited nucleation that couples the stochastic nature of cluster evolution with the evolving diffusion fields near the cluster has been refined. New methods for solving the large set of stiff, coupled, differential equations have allowed calculations of the time-dependent nucleation rate to be carried out to experimentally accessible times. In contrast with earlier theoretical studies, calculation results suggest a different dependence of the steady state nucleation rate and induction time on the diffusion rate in the initial glass phase. This can have a profound influence on the expected microstructures of solidified phases.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 4/96 EXPIRATION: 4/97

PROJECT IDENTIFICATION: 962-21-30

NASA CONTRACT NO.: NCC8-85

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Kelton, K.F. "Analysis of Crystallization Kinetics (Invited Talk)." Proceedings of the Ninth International Conference on Rapidly Quenched Metals, Bratislava, Slovakia (1996) (to appear in Mat. Sci. and Eng.).

Kelton, K.F. "Nucleation (Invited Talk)." Proceedings of summer school: Phasenubergänge in Metallen, Institut für Raumsimulation, DLR, Cologne, Germany, June 4-5, 1996.

Kelton, K.F. "Phase Formation and Stability: Composition and Sample-Size Effects." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Presentations

Kelton, K.F. "From Liquids to Crystals." Distinguished Lecture Series, Arkansas Tech University, Russellville, Arkansas, April 1996.

Lakshmi Narayan, K., and Kelton, K.F. "Crystallization Behavior in $\text{Na}_2\text{O} \cdot 2\text{CaO} \cdot 3\text{SiO}_2$ Glasses." Meeting of the American Physical Society, St. Louis, Missouri, April 1996.

Solutocapillary Convection Effects on Polymeric Membrane Morphology

PRINCIPAL INVESTIGATOR: Dr. William B. Krantz

University of Colorado, Boulder

CO-INVESTIGATORS:

Todd, P.
Owen, R.University of Colorado
Owen Research

Task Objective:

- Design experiments for casting polymeric membranes under low-g conditions to study the influence of solutocapillary convection effects on membrane structure.
- Utilize the low-g environment provided by the KC-135 aircraft in order to conduct experiments to discriminate between two hypotheses which have been advanced to explain macrovoid-pore formation in polymeric membranes.
- Modify and couple an exiting model developed for the dry-cast membrane formation process to a model for macrovoid growth caused by solutocapillary convection.

Task Description:

In order to study the influence of solutocapillary convection on polymeric membrane morphology and to discriminate between the two hypotheses advanced to explain the growth of macrovoids in the dry- and wet-cast membrane-formation processes, the following tasks are identified:

1. Specification of membrane-casting solutions
2. Design and construction of the test cells
3. Perform ground-based control experiments
4. Carry out low-g experiments in KC-135 flights
5. Carry out structural characterization of membranes
6. Model development

Task Significance:

Polymeric membranes are used for a variety of purposes ranging from water purification to environmental cleanup of effluent streams. Membranes remove impurities because of submicroscopic pores. One problem in creating submicroscopic pores in membranes is the propensity to form large pores or macrovoids which "short-circuit" the membrane's ability to separate dissolved impurities. Optimal means for eliminating macrovoids have yet to be developed owing to our lack of knowledge of what causes them. This research exploits the unique low-g environment to discriminate between two hypotheses advanced to explain macrovoid formation. The results of this research should enhance our ability to eliminate these undesirable defects during membrane manufacture.

Progress During FY 1996:

The following progress has been made in addressing this task:

1. Specification of membrane-casting solutions - The composition range of the casting solutions (cellulose acetate, acetone, water) has been determined to satisfy the criteria of low-gravity experimentation: macrovoid formation occurs, and phase inversion occurs in less than 20 seconds. Steps have been added to the preparation of the solutions, namely controlling water content using molecular sieves and controlling polymer molecular weight using ultracentrifugation, in order to make the solutions stable and predictable.

2. Design and construction of the test cells - Four flight-qualified test cells were constructed. Each membrane-casting apparatus (MCA) is capable of automatically casting 6 membranes 1 cm in diameter having depths ranging from 80 to 259 μm . Mass transfer of evaporating acetone is extremely rapid, being driven down a steep gradient by adsorption to a 100-fold excess of activated carbon. The exact transfer rate is being determined from a modified comprehensive model. The reaction is initiated by pulling a trigger and allowing a sliding block to spread the casting solution during a period of several milliseconds. Phase inversion occurs in less than 20 seconds, and the membranes are subsequently dried. This process is tracked by optical monitoring using a bifurcated fiber optic and measuring reflected light from the surface of the casting cell. The fiber-optic data are accumulated simultaneously with g-sensor and parabola-count data on a personal computer. This real-time measurement capability for studying membrane formation in low-g is novel and represents an added feature which we did not anticipate in our original proposal. It has added significantly to the value of the data.

3. Perform ground-based control experiments - Numerous membranes have been cast in the laboratory using the MCA's, and the conditions for forming macrovoids, as evaluated by scanning electron microscopy (SEM), are reproducible.

4. Carry out low-g experiments in KC-135 flights - Mr. Konagurthu completed all of the pre-flight physiological and medical procedures and is qualified to perform experiments on NASA's KC-135 low-g aircraft. Subsequent to guidance from Dr. Owen and from the BioServe Space Technologies Center staff, he assembled supporting flight hardware and performed low-g experiments for three days. About 50 membranes were cast during low-g, 2-g and level flight. The results were clear: membranes cast in low-g were saturated with macrovoids, some of which completely perforated the membrane; membranes cast in 2-g were, according to our observations, lacking in macrovoids; membranes cast in level flight were the same as on the ground -- a moderate incidence of macrovoids. These results are consistent with our original suggestion that solutocapillary flow, and not diffusion, is the cause of macrovoid formation.

5. Carry out structural characterization of membranes - SEM has been used to quantitate the incidence of macrovoids and to seek any other unusual characteristics. The only usual characteristic observed so far is "tunneling macrovoids," those that completely penetrate the membrane resulting in a straight hole from one side to the other.

6. Model development and corroboration - A coupled heat- and mass-transfer model has been developed in conjunction with the experimental research. It consists of a combined FORTRAN code by Shojaie and SPRINT subroutines by Berzins. It has been adapted to account for heat and mass transfer in low g, and also the physical casting conditions. The model predictions were corroborated using the reflectometry data obtained and also via a laser interferometry technique developed specifically for the MCA casting mechanism. The interferometry experiments were conducted in order to obtain instantaneous film thickness changes as a function of time, and the model predictions agreed quite well with the experimental data.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/94 **EXPIRATION:** 6/96

PROJECT IDENTIFICATION: 962-26-08-15

NASA CONTRACT NO.: NAG8-106

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Konagurthu, S., Krantz, W.B., Greenberg, A.R., and Todd, P. "A Novel Approach to Test Alternative Hypotheses for Macrovoid Growth in Polymeric Membranes." Eighth Annual Meeting of the North American Membrane Society, Ottawa, Canada, May 1996 (the NAMS technical committee awarded first place for the best student paper).

Influence of Natural Convection and Thermal Radiation on Multi-Component Transport and Chemistry in MOCVD Reactors

PRINCIPAL INVESTIGATOR: Dr. Anantha Krishnan

CFD Research Corporation

CO-INVESTIGATORS:

Lowry, S.
Clark, I.O.CFD Research Corporation
NASA Langley Research Center (LaRC)

Task Objective:

The main objective of the proposed study is to quantify and assess the influence of natural convection coupled with non-convective phenomena in a Metalorganic Chemical Vapor Deposition (MOCVD) system over a range of Gr/Re^2 numbers for different inlet flow conditions, substrate temperatures, reactor pressures and reactant compositions.

Task Description:

The proposed work involves the collaboration between CFDRC and NASA LaRC in performing computational and experimental studies of the MOCVD system at NASA LaRC. CFDRC's commercial code, CFD-ACE, will be applied to simulate the MOCVD system over a range of operating conditions.

The technical approach is as follows:

1. Perform parametric studies with the numerical model for a matrix of boundary conditions and gravity levels.
2. Perform closely coupled ground-based experiments to validate the model predictions.
3. Conduct extensive parametric studies (following model validation) to optimize growth process under ground-based conditions.
4. Extrapolate ground-based simulations to microgravity.

Task Significance:

MOCVD is a commonly used technique for growing III-V and II-VI compound semiconductors and alloys. Despite its widespread use, the inherently complex transport and chemistry mechanism associated with MOCVD are not well understood. In this regard, it is important to understand the individual roles of various physical phenomena and operating conditions on the growth process. Of these phenomena, the influence of natural convection is one of the least quantified and understood. Improved understanding of the process, including the effects of natural convection, can be used to identify conditions that result in improved growth structures and process efficiencies.

Both forced and natural convection are present in ground-based MOCVD systems. Buoyancy driven convection arises due to density variations created by thermal and concentration gradients inherent to the process. Natural convection creates composition and thermal non-uniformities that translate into non-uniformities in the substrate composition and growth rate. Natural convection also makes it difficult to isolate and analyze fundamental non-convective transport and reaction mechanisms.

Progress During FY 1996:

This project was begun on May 28, 1996 and the progress for the first quarter (May 28, 1996 - August 28, 1996) is described below. The work plan for the first year focuses on experimental and computational studies (with pure fluids such as nitrogen and hydrogen) to analyze the effects of radiative heat transfer on natural convection. The technical progress achieved during the first quarter is as follows:

The initial simulations were oriented towards obtaining a basic understanding of the interaction between thermal radiation and natural convection in channel flows. Three-dimensional flow of nitrogen in a rectangular channel (with one heated wall) was analyzed. Gravitational effects were considered in the model. Simulations were performed with and without the radiation model to assess the effect on the extent of natural convection in the channel. For this problem, it was found that radiation has a significant role in altering the thermal boundary

conditions in the channel. Specifically, the altered boundary conditions resulted in a reduced effect of natural convection.

The geometry and experimental data (velocity and temperature distributions) on the LaRC MOCVD reactor have been transferred to CFDRC. A three-dimensional, non-orthogonal model (based on body-fitted-coordinates) of the reactor has been created to simulate the geometrical boundary conditions accurately. Preliminary simulations have been performed using the model. The results are currently being analyzed and will be discussed in detail in the next report.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 **EXPIRATION:** 6/00

PROJECT IDENTIFICATION: 962-21-19

NASA CONTRACT NO.: NAS8-408

RESPONSIBLE CENTER: MSFC

Containerless Property Measurement of High-Temperature Liquids

PRINCIPAL INVESTIGATOR: Dr. Shankar Krishnan

Containerless Research, Inc.

CO-INVESTIGATORS:

Nordine, P.C.

Containerless Research, Inc.

Task Objective:

The task objective is to measure the optical properties of high-purity liquid metals and alloys (Al, Zr, Ni, and Ni-Zr alloys) over wide wavelength (220–1100 nm), temperature ($T_m + 300$ K), and composition ranges under containerless conditions. Spectroscopic, pulsed dye-laser ellipsometry is used to obtain the complex dielectric functions and spectral emissivity data at high temperatures on clean liquids using electromagnetic levitation. These data are needed for accurate noncontact temperature measurement, and for measurements of the total hemispherical emittance by integration of emissivity over the wavelength range of thermal emission.

Another major outcome of this research will be the determination of the optical properties of liquids over a wide wavelength range. These measurements are of fundamental importance to advancing the theory of liquid metals. For example the presence or absence of important interband transitions provides information on the valence, bonding, joint density-of-states, and the extent to which nearly-free electron behavior is exhibited by liquid metals and alloys.

Task Description:

The research approach is to levitate liquid metals and alloys (Al, Ni, Zr, and Ni-Zr alloys) electromagnetically and use a spectroscopic pulsed dye-laser ellipsometer to measure the complex dielectric function and the spectral emissivity in the wavelength range 220–1100 nm. Pulsed radiation is generated by a Molelectron dye-laser, and the wavelength is automatically set and adjusted by a laboratory computer. Light reflected by the specimen is collected and analyzed by a unique rotating analyzer ellipsometer.

The rotating components of the ellipsometer are motorized and controlled by the computer. The signals are detected by a pair of photodiodes and an EG&G boxcar averager is used to extract the mean value of the light intensities at the two photodiodes which receive the orthogonally polarized components of the reflected light. The signals are automatically measured by the computer.

A Molelectron dye laser is used to generate pulsed radiation in the 220–1100 nm wavelength range. The light is steered through several mirrors, and transmitted through a pair of Glan Thomson linear polarizers. The second polarizer is fixed in azimuth, and rotation of the first polarizer allows light levels to be adjusted to the optimum values. The light is incident on the liquid specimens at a fixed incident polarization, and the reflected polarization is analyzed for its new azimuth and ellipticity.

A modified rotating analyzer ellipsometer is used to measure the outgoing polarization at 6 azimuths of the analyzer. The analyzer is of the beamsplitting type such that the two orthogonal components of the beam are simultaneously obtained. Three intensity ratios are measured at three independent pairs of azimuths. The complex dielectric constant, indices of refraction, and spectral emissivities are derived from standard equations. The light intensities are detected by a pair of high speed, UV-enhanced silicon photodiodes and measured by a pair of gated integrators.

The emphasis of measurements on liquid metals and alloys is to determine the temperature and (for alloys) composition dependence of all optical properties over the accessible wavelength range. Measurements are possible from approximately 0.8 of the melting temperature, (T_m) in undercooled liquids to at least 300K above T_m . The observed effects of temperature and composition on optical properties and the wavelength dependence of these properties are interpreted in terms of liquid structure and bonding.

The liquid nickel, zirconium, and their alloys have been chosen to be investigated in this research because they display unique glass forming behavior, typify early and late transition metals, and because they are also of interest

to other NASA investigators. Measurements at 633 nm on these metals is being conducted in collaboration with Professors Bayuzick of Vanderbilt University and Johnson of the California Institute of Technology.

Task Significance:

The relevance and significance to the microgravity program are twofold. First, the spectral emissivity and total hemispherical emissivity form the basis for new noncontact thermophysical property measurements in microgravity experimentation. For example, knowledge of total hemispherical emittance allows heat capacity and thermal diffusivity to be accurately determined from free-cooling and pulse-heating experiments. Spectral emissivity data allow true specimen temperatures to be determined using optical pyrometry. Second, spectral emissivity measurements on specific materials are needed by other NASA investigators in ground-based and microgravity experimentation.

Progress During FY 1996:

During the past year, work has continued towards optical property measurements on liquid metals and alloys. Materials investigated include liquid Ni, Fe, Ni-75%Zr, and some of the materials investigated by other PI's on the TEMPUS experiments. The optical properties including the complex dielectric function and the spectral emissivities for these liquid materials have been measured in the wavelength range of 360-1000 nm (1-4 eV) and at selected wavelengths as functions of temperature. Based on these results, some modelling has also been conducted to extract approximate values of the total hemispherical emissivity needed in the analysis of heat transfer. A few papers and presentations summarizing the results have also been made. During this last year of performance, two NRA proposals have been submitted for continuing work in the area of optical and thermophysical property measurements. Work has also continued to disseminate results obtained in our laboratory over the past year, in the form of three new publications.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/92 EXPIRATION: 5/96

PROJECT IDENTIFICATION: 963-25-07-05

RESPONSIBLE CENTER: JPL

Noise and Dynamical Pattern Selection in Solidification

PRINCIPAL INVESTIGATOR: Prof. Douglas A. Kurtze

North Dakota State University

Co-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

To understand the fundamental mechanisms by which a pattern-forming system can change the spacing of its pattern, and to devise a means of calculating the preferred spacing to which external noise will drive the pattern.

Task Description:

Numerical computation of the time evolution of mathematical models of solidification fronts, and analytical arguments to extract the preferred spacing from the model equations are both aspects of this task.

Task Significance:

Properties of materials grown from the melt are largely determined by their microstructure, which in turn is strongly affected by the front shape during solidification. This research will establish whether processing in a noisy environment (such as the Space Shuttle) can lead to more reproducible, and hence better controlled, front shapes than processing in a quieter environment. This study will definitively enhance our understanding of the fundamentals of solidification. A more complete study (such as this) is required for the design of materials with specific materials properties; a difficult task, but an important practical goal.

Progress During FY 1996:

Work based on the Fokker-Planck equation for pattern forming systems driven by white noise has shown that there is one state of such a system, among all its possible stable steady states, which is preferred, in the sense that weak noise will cause it to spend most of its time near that state. Calculating this preferred state involves solving an associated classical mechanics problem, and is beset by difficulties coming from the fact that this classical mechanics problem is in general non-integrable. It seems more promising to approach the problem numerically, with small but finite noise strength, rather than working analytically in the weak-noise limit. In order to do this, I have developed a path integral formulation for solving the Fokker-Planck equation with arbitrary noise strength, and I am currently working on a numerical methods for implementing it.

Two more analytical approaches to the problem are under way. One is to look at the possibility of using perturbation methods to solve problems which are close to having an underlying free energy. This would be relevant to pattern-forming systems which are just beyond the onset of instability of the simple basic shapes, which is the only regime for which general analytical results of any kind are valid. This approach has led to some results for simplified models of Rayleigh-Benard convection. The other is to investigate whether there is a connection between the correct Fokker-Planck results and a more heuristic argument based on the tendency of peaks in the systems spectrum to move in a direction which can be calculated from the system's evolution equations.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 0

TASK INITIATION: 10/94 EXPIRATION: 10/96

PROJECT IDENTIFICATION: 962-25-05-30

NASA CONTRACT NO.: NAG3-160

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Kurtze, D.A., Noise and dynamical pattern selection. Phys. Rev. Lett., 77, 63 (1996).

Study of Magnetic Damping Effect on Convection and Solidification under G-Jitter Conditions

PRINCIPAL INVESTIGATOR: Dr. Ben Q. Li

Louisiana State University

CO-INVESTIGATORS:

de Groth III, H.C.

NASA Lewis Research Center (LeRC)

Task Objective:

As shown by NASA resources dedicated to measuring residual gravity (SAMS and OARE systems), g-jitter is a critical issue affecting space experiments on solidification processing of materials. This newly-funded study aims to provide an assessment of the use of magnetic fields in combination with microgravity to reduce the g-jitter induced flow in space. The objectives of this research project are threefold: (1) to determine the behavior of g-jitter induced convection in a magnetic field; (2) to assess the abilities of magnetic fields to suppress the detrimental effects of g-jitter during solidification; and, (3) to develop an experimentally verified numerical model capable of simulating transport processes and solidification phenomena under g-jitter conditions with and without a magnetic field. The FY96 task objectives involve developing a 2-D mathematical model for g-jitter driven flow and constructing and testing a ground-based physical model by which numerical modeling results will be compared and verified.

An experimental setup will be built and mercury will be used as a testing fluid. The oscillating flow, which is intended to simulate the effect of single frequency g-jitter, is generated in the mercury by applying an oscillating temperature boundary condition. External magnetic fields are applied and their effects on the damping of the oscillating convective flows will be studied. The flow velocities in the mercury pool will be measured using hot film anemometers with and without the presence of an applied magnetic field. These experiments are intended to provide a basic understanding of the behavior of the gravity-induced oscillating convective flow with and without an applied magnetic field. Further experiments of magnetic damping during unidirectional solidification will be conducted in NASA's magnetic damping furnace at the NASA Lewis Research Center. Both the laboratory and NASA's Lewis magnetic damping experiments will be used to verify and refine numerical models, as described below, and to assess the effectiveness of a magnetic field in damping the deleterious effects associated with g-jitter.

Task Description:

The theoretical part of the FY96 objectives entails developing a 2-D finite element model to represent the complex transport phenomena associated with magnetic damping during solidification in space, such as the induced Lorentz force distribution, fluid flow and temperature distribution in melts under g-jitter conditions. The numerical model will be developed based on our existing finite element code for fluid flow and heat transfer calculations. With the model, the melt flow behavior under the influence of a magnetic field will be studied as a function of operating conditions for space experiments, including (1) gravity orientation, (2) magnetic field strength, and (3) oscillation frequency. To test and verify the model predictions, an experimental setup will be built and mercury will be used as a testing fluid. The oscillating flow, which is intended to simulate the effect of single frequency g-jitter, is generated in the mercury by applying an oscillating temperature boundary condition. External magnetic fields are applied and their effects on the damping of the oscillating convective flows are studied. The flow velocities in the mercury pool will be measured using hot film anemometers with and without the presence of an applied magnetic field. The measurements will be used to verify and refine the numerical model predictions.

Task Significance:

While there has been research on the understanding of deleterious g-jitter effects on convective flow during solidification processes, little work has yet been reported on the application of magnetic damping to suppress the g-jitter induced flow in microgravity. This project, specifically addressing this problem through a combined approach of mathematical modeling and ground-based physical simulation and solidification experiments, will have significant impact on our fundamental understanding of the interactive nature of magnetic fields and transport phenomena under g-jitter conditions in microgravity. The information developed from the numerical simulations and experiments will create a rational basis for the development of microgravity magnetic damping facilities for space applications. The numerical models and experimental setup will also have the potential of serving the users of magnetic damping facilities in planning experiments under microgravity conditions and interpreting the measured results obtained in space.

Progress During FY 1996:

This research project was funded starting June 1996. So only some preliminary aspects of the program have gone forward in the past fiscal year. In the FY96 time frame, we have started to purchase necessary equipment and started to develop numerical models. Some of the preliminary results were presented in a Microgravity Materials Science Conference poster presentation. One journal paper was written and was sent for review. Currently, our focus is on the developing numerical models and establishing laboratory system for the study of magnetic damping effects on microgravity fluid flows.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 6/96 **EXPIRATION:** 5/00

PROJECT IDENTIFICATION: 962-21-40

NASA CONTRACT NO.: NCC8-92

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Li, B.Q., and de Groh, H.C. "Study of Magnetic Damping Effect on Convection and Solidification under G-Jitter Conditions (poster presentation)." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Microstructural Development during Directional Solidification of Peritectic Alloys

PRINCIPAL INVESTIGATOR: Dr. Thomas A. Lograsso

Iowa State University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The mechanisms of and conditions required for the formation of peritectic solid dendrites, cells, or planar growth between the primary solid dendrites or cells and the transitions between these structures will be investigated. In addition, alternating bands of solid phases perpendicular to the growth direction have been observed in peritectic systems. However, the precise conditions under which these bands form and the mechanisms by which these bands form are not clearly understood. It has been postulated that the development of these different structures is related to changes in the composition of the liquid. A model has been developed that predicts the compositional variations that occur in the liquid under the assumption of no convection. This model has been compared to experimental results to clarify the formation mechanism and to evaluate the importance of convective effects on the formation of various structural characteristics.

Task Description:

This research will focus on:

1. Establishing the growth conditions in terms of temperature gradient and growth rate for the formation of planar, cellular, and dendritic growth of the peritectic solid in a two-phase peritectic under conditions of minimal convective flow, with an emphasis on the morphological transition from cellular front primary and planar front peritectic solid to single phase planar front solid; and,
2. Determining the effect of conditions of minimal convective flow on the formation of a banded structure during directional solidification of a two-phase peritectic alloy.

The research approach is to initially focus on two alloy systems, In-Sn and Sn-Cd. In-Sn has a very low peritectic temperature, which allows for the possibility of direct observation during solidification. In addition, In and Sn have essentially equal densities in the liquid state in the temperature range of interest, which should minimize density-driven convection. In the Sn-Cd system, the solute element (Cd) is more dense in the liquid state, which should minimize density-driven convection when solidification occurs upward. This system has been well characterized and is more tractable in terms of sample preparation than In-Sn. These results can be compared to previous work on the Pb-Bi system, in which the solute element (Bi) is less dense and thus provides a driving force for mixing in the liquid through convection.

Task Significance:

This research effort will establish the ground-based data required for the identification of the appropriate alloy system, composition, and growth conditions for microgravity processing. Studying solidification for these types of systems is important, because a number of industrially significant materials solidify in a similar manner such as brass, bronze, some steels and high temperature superconductors. The utilization of a microgravity environment greatly facilitates the analysis and modeling of data, since gravity-induced mixing in the liquid can strongly affect the solidification process.

Progress During FY 1996:

The research effort focused on directional solidification experiments using peritectic alloys of the Sn-Cd system and conditions which produced layered microstructures. Due to questions raised by the previous results, the composition of the peritectic phase at the peritectic temperature was measured. The value of this composition relative to the alloy composition being used experimentally supported the idea that the operative layer formation mechanism was different from that of the currently published model. The crystallographic orientation of adjacent layers was then determined. Since the orientation did not vary in two series of layers, the layers were most likely interconnected in three dimensions. This continuity indicated that the repetitive nucleation and growth described in the currently

published model was not required for the layer formation in these samples. An alternative formation mechanism based on competitive growth of the two solids at a mutual solid-liquid interface was proposed. Layer lengths were measured for other alloy compositions as a function of growth velocity to determine the effect of composition variations within the peritectic isotherm. Samples were also solidified in the presence of temperature oscillations in order to examine the effect of external perturbations on the formation of layers.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/93 EXPIRATION: 7/96

PROJECT IDENTIFICATION: 962-25-08-28

NASA CONTRACT No.: NAG8-963

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Zeisler-Mashl, K.L., and Lograsso, T.L. Determination of the In-rich peritectic region in the In-Sn system by differential scanning calorimetry. *J. Phase Equilibria*, vol. 16, 516-519 (1995).

Zeisler-Mashl, K.L., and Lograsso, T.L. Measurement of the peritectic phase composition in the Sn-Cd system through directional solidification techniques. *J. Phase Equilibria*, vol. 17, 7-9 (1996).

Presentations

Zeisler-Mashl, K.L., and Lograsso, T.L. "Band formation during directional solidification in peritectic systems." 1995 TMS Fall Meeting, Cleveland, Ohio, October 1995.

Zeisler-Mashl, K.L., and Lograsso, T.L. "Microstructural development during directional solidification of peritectic alloys." Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.

Zeisler-Mashl, K.L., Lograsso, T.L., and Trivedi, R.K. "The influence of convection on banding in peritectic systems: a comparison of Sn-Cd and Pb-Bi." 8th International Symposium on Experimental Methods for Microgravity Materials Science, Anaheim, California, February 1996.

Numerical Investigation of Thermal Creep and Thermal Stress Effects in Microgravity Physical Vapor Transport

PRINCIPAL INVESTIGATOR: Dr. Daniel W. Mackowski

Auburn University

CO-INVESTIGATORS:

Knight, R.

Auburn University

Task Objective:

The objective of this research is to quantitatively predict the roles of thermal creep and thermal stress on microgravity physical vapor transport through detailed numerical calculations.

Task Description:

The research will formulate thermal creep and stress effects into a variable property, two-dimensional representation of heat and mass transfer in cylindrical ampoules under typical operating parameters. Physical conditions at which thermal creep and stress significantly alter vapor transport from a pure diffusion-limited mode, as well as the resulting effects upon mass transfer rates and mass flux uniformity at the crystal surface, will be determined. The research will benefit the prediction and development of microgravity crystal growth technology by providing, for the first time, an accurate accounting of all relevant physical vapor transport mechanisms.

The potential for growing high-quality crystals in closed, cylindrical ampoules using chemical vapor transport and physical vapor transport processes under microgravity conditions has been demonstrated in a number of experiments. The development of this technology will require an accurate modeling of the relevant vapor transport mechanisms occurring in buoyancy-free environments. Previous numerical efforts to predict microgravity crystal growth rates have employed a diffusion-limited formulation of vapor transport. However, theoretical arguments strongly indicate that the non-isothermal conditions encountered in ampoules can lead to an appreciable motion of the bulk fluid as a result of previously unrecognized phenomena. Temperature gradients tangential to the ampoule side walls can, through the mechanism of thermal creep, drive a slip flow of gas over the surface. In addition, temperature gradients within the gas itself can induce a fluid stress, and resulting fluid motion, through the mechanism of thermal stress. Order-of-magnitude estimates suggest that, under typical ampoule conditions, the fluid velocities resulting from thermal creep and thermal stress can be comparable to vapor diffusion velocities.

Specific tasks include:

- Develop code for numerically solving governing differential equations. Assemble thermodynamic and transport property database of commonly used PVT samples and carrier gases.
- Perform numerical calculations of diffusion-buoyant convection vapor transport in the absence of thermal creep and thermal stress. Check numerical results with previously published results.
- Incorporate thermal creep boundary conditions and thermal stress constitutive law into numerical code. Determine model parameter values at which thermal effects significantly alter vapor transport from diffusion and buoyant convection predictions.
- Determine the individual effects of thermal creep and thermal stress on vapor mass transport rates and the uniformity of mass flux at the crystal surface. Based on numerical results, develop rational expressions for estimating the relative contributions of the thermal vapor transport mechanisms to mass flux as a function of ampoule, sample, and carrier parameters.

Task Significance:

Under earthbound conditions, heat and mass transfer within nonisothermal physical vapor transport (PVT) crystal growth ampoules will often be dominated by buoyant convection. The rationale for performing PVT experiments in microgravity conditions is that the buoyant convective mechanisms will be suppressed, and crystal growth will occur in a diffusion-limited mode. However, qualitative arguments indicate that the convective mechanisms of

thermal creep and thermal stress, which are usually negligible in comparison to buoyant convection in earthbound environments, could significantly effect mass transfer rates in microgravity PVT systems. A quantitative understanding of the role of these mechanisms in microgravity PVT crystal growth processes requires detailed numerical modeling.

Progress During FY 1996:

The final efforts of this project were focused on examining convection in nonisothermal gases that result from thermal stress. Thermal stress is predicted from the Burnett contributions to the fluid stress tensor, which constitute the second-order approximation to the Boltzmann equation for small Knudsen flows (the Navier-Stokes equations being the first order approximation).

Inclusion of the Burnett terms into the Navier-Stokes equations have been shown to increase the accuracy of continuum-based CFD models when applied to transitional Knudsen regimes and highly nonequilibrium conditions (such as in hypersonic flows). However, there are several unresolved theoretical issues regarding the validity and accuracy of the Burnett terms (e.g., convergence in Knudsen number, solution uniqueness, and validation of Second-Law principles). Precise experimental measurements of the effects of thermal stress on gas flows would provide valuable information towards the understanding of the Burnett terms. Such measurement, however, are difficult to perform under earthbound conditions, primarily because thermal stresses become small relative to fluid shear (in high speed flow) or buoyant forces (in low speed flow).

Controlled measurements of thermal stress convection could, in principle, be performed in the microgravity environment. We have numerically calculated flowfields, using the continuum formulation (Navier-Stokes + Burnett with slip and jump-corrected boundary conditions) for a monatomic gas contained within a nonuniformly heated enclosure. Under buoyancy-free conditions, our calculations indicate that temperature gradients on the order of 200 K/cm can lead to a measurable recirculation of a gas (e.g., velocities on the order of 1 cm/s for atmospheric pressure conditions). Heating and containment strategies which maximize the thermal stress flows, and measurement of flow velocities via particle tracking methods, have been examined. We are also in the process of comparing flow fields calculated from the continuum formulation (Navier-Stokes + Burnett) with those obtained from Direct-Simulation-Monte-Carlo solutions to the Boltzmann equation.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/93 EXPIRATION: 1/96

PROJECT IDENTIFICATION: 962-21-08-18

NASA CONTRACT NO.: NAG8-977

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Mackowski, D.W., and Knight, R.W. Numerical investigation of thermal creep and thermal stress effects in microgravity physical vapor transport, Final Technical Report for NASA contract NAG8-977. Auburn University, Department of Mechanical Engineering, (January 1996).

Mackowski, D.W., Rao, V.R., and Knight, R.W. Effect of solid phase heat transfer and wall deposition on crystal growth in physical vapor transport ampoules. J. of Cryst. Growth, vol. 165, 323-334 (1996).

Presentations

Mackowski, D.W., and Knight, R.W. "Investigation of thermal stress convection in nonisothermal gases under microgravity conditions." Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 1996 (NASA Conference Publication 3338).

Polymerizations in Microgravity: Traveling Fronts, Dispersions, Diffusion and Copolymerizations

PRINCIPAL INVESTIGATOR: Dr. Lon J. Mathias

University of Southern Mississippi

CO-INVESTIGATORS:

Lochhead, R.

University of Southern Mississippi

Pojman, J.

University of Southern Mississippi

Task Objective:

Polymerization studies of bulk-phase diffusion and polymerization in monomer and co-monomer mixtures or in monomer droplets in a non-solvent are being performed to study density effects on polymerization.

Task Description:

These experiments will allow determination of fundamental monomer and polymer properties. The diffusion rate constants to be measured in the absence of convective mixing have not been accurately measurable on earth. This data will provide new insights into the fundamental behavior of polymers in a variety of situations important to their formation and processing. For example, molecular weights and distributions are directly dependent on the relative diffusion behavior of monomers and polymers. Processing of polymers, either in solution or from the melt, involves molecular reorganization and motion. The combination of convective mixing with diffusion determines the ability of polymers to effectively orient into crystalline domains. A further example is provided by co-polymerizations at high conversion. In this regime, which is industrially important on Earth, the diffusion constants of monomers and polymers become extremely important. The co-polymer composition throughout the reaction must be amenable to calculation and prediction. This is currently not possible without accurate knowledge of polymer and monomer diffusion constants.

Three separate but closely related research investigations are being conducted that all deal with developing a fundamental understanding of monomer and polymer diffusion during polymerization or processing under widely different conditions, and with applying this knowledge to the formation of unique materials. The three projects all involve bulk-phase diffusion and polymerization in neat monomer or co-monomer mixtures, or in monomer droplets dispersed in nonsolvent. All three deal with diffusion effects that should uniquely manifest themselves under microgravity where analysis by optical, interference and light scattering will give complete understanding of macroscopic down to molecular level behavior.

Task Significance:

Microgravity offers a unique environment for studying polymer diffusion and polymer polymerization reactions. The absence of convection currents, which are the major mode of mixing at the molecular level on earth, are eliminated or reduced in the microgravity environment. More importantly, the prediction of unique co-polymer composition development in microgravity will allow controlled formation of new compositions of matter. The absence of mixing at the molecular level should produce unique short-block co-polymers available for the first time for co-monomer compositions which normally lead to random or long-block co-polymers under good mixing.

Progress During FY 1996:

Significant progress was made during the year on both ground-based and flight experiments. Despite the fact that our project is just over three years old, we have not only developed sufficient ground-based data to design experiments for microgravity, but we have actually carried out a number of flight experiments and have developed hardware and schedules for additional flight experiments during the coming years. Flight experiments include:

- KC-135 homopolymerizations of methyl methacrylate which showed significantly higher molecular weights in microgravity than on earth. A reflight of this was carried out in August 1996 to obtain microgravity (1.8 g) control samples. A repeat is planned in December 1996 for correlation of results with light intensity and gravity.
- A GAS can experiment (combined Code C/Code U effort) returned in September 1995 from the Space Shuttle in which several types of polymerizations were evaluated. Preliminary results confirm successful reaction although detailed analysis must still be done.

• A sounding rocket experiment (combined Code C/Code U effort) was carried out and preliminary results are being summarized for publication.

• Several industrial sponsors were lined up for Code C sponsorship of the 3M Gosmar rapid mixing reactor. Experiments will involve polyaniline single crystal formation (IBM collaboration) and several experiments with sterically stabilized polymer dispersions (GE and Calgon main sponsors). This will be designated for Shuttle flight in the next 12-18 months.

Ground-based work has been as extensive as our flight efforts. Specifically, we have accomplished much in all three components of the project:

• Developed a series of new monomers for photopolymerization which are much faster than other methacrylates and that will allow detailed evaluation of homo- and co-polymerization studies in microgravity using both thermal and photoinitiation.

• Evaluated the role of polymerization fronts in developing new compositions of matter such as composites, filled and reinforced thermosets, and thermally generated two-component interpenetrating polymer networks.

• Carried out detailed evaluation of the absorption of hydrophobically-modified polymers at oil-water interphases during extremely slow (15 hour) quiescent conditions as well in rapid experiments in a turbulent flow regime. It was confirmed that a critical Reynold's number must be attained to allow absorption of the polymers to confer emulsion stability. Experiments were carried out under isopycnic conditions to mimic microgravity.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 3

TASK INITIATION: 4/93 **EXPIRATION:** 10/95

PROJECT IDENTIFICATION: 962-26-08-10

NASA CONTRACT NO.: NAG8-973

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Avci, D., and Mathias, L.J. Cyclopolymerization of Cinnamate Ester Derivates of Alkyl α -(Hydroxymethyl) Acrylates. *Polymer Bulletin*, vol. 35, 671 (1995).

Avci, D., and Mathias, L.J. Examples of New Synthetic Routes to Pendant Ester-Ether Derivatives of α -Hydroxymethylacrylate Polymers. *Polymer Bulletin*, vol. 3, no. 2, 133 (1996).

Avci, D., Thigpen, K.T., and Mathias, L.J. Effects of Reduced Gravity on the Molecular Weight of Photopolymerized Methyl Methacrylate. *Polymer Preprints*, vol. 37, no. 2, 317 (1996).

Avci, D., Thigpen, K.T., and Mathias, L.J. Photopolymerization Studies of Alkyl and Aryl Ester Derivatives of Ethyl α -Hydroxymethylacrylates. *J. Poly. Sci., Polym. Chem. Ed.*, vol. 34, no. 5, 3191 (1996).

Khan, A.M., and Pojman, J.A. The Use of Frontal Polymerization in Polymer Synthesis. *Trends in Polymer Science*, vol. 4, 253 (1996).

Mathias, L.J., Thigpen, K.T., and Avci, D. Superfast Methacrylate Photomonomers: Aryl Ester Derivatives of Ethyl α -Hydroxymethylacrylates. *Macromolecules*, vol. 28, 8872 (1995).

Pojman, J.A., Ilyashenko, V.M., and Khan, A. Free-Radical Frontal Polymerization: Self-Propagating Thermal Reaction Waves. *J. Chem. Soc., Faraday Trans.*, vol. 92, 2824 (1996).

Presentations

Avci, D., Thigpen, K.T., and Mathias, L.J. "Effects of Reduced Gravity on the Molecular Weight of Photopolymerized Methyl Methacrylate." ACS National Meeting, Orlando, Florida, August 25-29, 1996.

Khan, A., and Pojman, J.A. "Frontal Polymerization of n-Butyl Acrylate." ACS National Meeting, New Orleans, Louisiana, March 24-28, 1996.

Pojman, J.A. "Frontal Polymerization: Quo Vadis?" ACS National Meeting, New Orleans, Louisiana, March 24-28, 1996.

Pojman, J.A. "Frontal Polymerization: From Dynamics to Materials (invited presentation)." 28th Congres National D'Analyse Numerique, La Londe-Les Maures, France, May 29, 1996.

Pojman, J.A., and Khan, A. "Reactor Design and Performance for the Study of Frontal Polymerization." ACS National Meeting, Orlando, Florida, August 25-29, 1996.

Pojman, J.A., Fortenberry, D., Khan, A., and Ilyashenko, V.M. "Frontal Polymerization: Self-Propagating High Temperature Synthesis (SHS) of Polymeric Materials." ACS National Meeting, Orlando, Florida, August 25-29, 1996.

Pojman, J.A., Gilla, N., Willisa, J., and Whitehead, J.B. "Polymer Dispersed Liquid Crystal (PDLC) Materials Produced via Frontal Epoxy Curing." ACS National Meeting, Orlando, Florida, August 25-29, 1996.

Quantitative Analysis of Crystal Defects by Triple Crystal X-Ray Diffraction

PRINCIPAL INVESTIGATOR: Dr. Richard J. Matyi

University of Wisconsin, Madison

CO-INVESTIGATORS:

Gillies, D.

NASA Marshall Space Flight Center (MSFC)

Task Objective:

The objective of this task involves the development of various x-ray diffraction methods for the analysis of semiconductor materials, particularly II-VI semiconductors. The specific goals are: (1) the development of high resolution triple crystal x-ray diffraction methods for the quantitative analysis of structural defects in semiconductor crystals; (2) the application of these analytical methods to compound semiconductor crystals (grown both in ground-based experiments, and eventually, in microgravity) to achieve a better understanding of the effects of the crystal growth environment on the generation of defects; and, (3) the transfer of this analysis technology to the Space Science Laboratory at the Marshall Space Flight Center (MSFC).

Task Description:

The overall investigative approach of the research is the coupling of a new materials characterization tool (triple crystal x-ray diffraction) to the development of a new crystal growth system. Various II-VI semiconductor samples are being supplied by MSFC and are currently being analyzed by triple crystal diffraction methods to articulate the mosaic structure and the density of statistically distributed dislocations. Diffuse scattering is being used to monitor the surface preparation. Plans are being made to investigate the use of anomalous transmission as an alternate means of characterizing the defect structure, and to measure the volume fraction of twinned material using x-ray methods. The information obtained in these analyses is being forwarded to MSFC for corroboration by other analytical methods.

Task Significance:

The Microgravity Science and Applications Division at the Marshall Space Flight Center is engaged in a program under an approved flight experiment for the growth of II-VI semiconductors in space. Of prime importance in any crystal growth process is the reduction of the density of grown-in structural defects and the understanding of the relation between crystal growth and defect generation. Recent research at the University of Wisconsin - Madison has demonstrated that an analytical technique known as triple-crystal x-ray diffraction is capable of clearly differentiating the defect-free, "perfect crystal" regions of a sample from regions that are structurally defective. In this research program, we will use triple-crystal x-ray diffraction and related methods to examine the evolution of crystal growth defects as a function of crystal growth and relate the nature and quantity of these defects to the growth process. This differentiation and measurement of the effect of defects will be used to give a clearer insight into the effects of microgravity on the growth of technologically-important crystals.

Progress During FY 1996:

Our experimental work has concentrated on developing and demonstrating HRTXD methods of characterizing crystals grown both on earth and in microgravity. The diffracted intensity about the 333 reciprocal lattice point from a sample of CdZnTe grown on USML-1 showed a roughly symmetric distribution of diffuse intensity about the 333 point; this is indicative of a relatively isotropic distribution of dislocations in the diffracting volume. In addition, a well-defined crystal truncation rod, or surface streak, was observed extending perpendicular to the surface. The presence of a well-defined surface streak indicates that the bulk crystal has sufficient structural perfection in order to diffract dynamically, and that the crystal surface is of high enough quality to produce the surface streak at all. In contrast to the relatively perfect CdZnTe, a 111 reciprocal space map of a ZnTe sample grown at the MSFC revealed multiple surface streaks; this behavior is characteristic of a sample with large mosaic blocks that are relatively perfect (low in dislocation density) but with a high degree of misorientation with respect to each other. Reciprocal space maps have also been obtained from ZnSe samples grown at MSFC. A ZnSe crystal with a cleaved [110] surface showed both a well-defined surface streak and a relatively large amount of diffuse scatter distributed perpendicular to the [110] surface normal direction. The diffuse scatter indicates a high dislocation density; however, the uniformity of this intensity suggested that the dislocations were randomly distributed throughout the crystal and not concentrated into subgrain boundaries. A reciprocal lattice map from a ZnSe sample with a polished

surface showed the complete absence of any surface streak, and both the intensity and the angular extent of the diffuse intensity indicated a highly defective surface region in this sample.

We have expended significant effort in developing a theoretical framework for calculating the effect of dislocations in bulk II-VI semiconductors on the diffuse x-ray scattering observed in high resolution triple crystal x-ray diffraction (HRTXD) measurements. In this approach we have adopted a model based in the kinematical theory for straight dislocations in which the Burgers vector is parallel to the $\langle 110 \rangle$ directions. The calculated diffuse scattering profile perpendicular to a reciprocal lattice vector has been compared with experimental intensity profiles recorded from the (333) reflection from CdZnTe and the (220) reflection from ZnSe. In the case of the CdZnTe, good agreement between the theoretical and experimental scattering curves were obtained for an assumed dislocation density in the range of $1 \times 10^5 \text{ cm}^{-2}$, while the ZnSe scattering profile was adequately fit with assumed density of $2 \times 10^7 \text{ cm}^{-2}$. We are currently working on refining this model through comparison with synchrotron topography data.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/94 EXPIRATION: 7/96

PROJECT IDENTIFICATION: 962-21-08-28

NASA CONTRACT NO.: NCC8-052

RESPONSIBLE CENTER: MSFC

Numerical and Laboratory Experiments on the Interactive Dynamics of Convection, Flow, and Directional Solidification

PRINCIPAL INVESTIGATOR: Prof. Tony Maxworthy

University of Southern California

CO-INVESTIGATORS:

Meiburg, E.

University of Southern California (USC)

Task Objective:

To determine, using experimental and numerical methods, the effects of externally imposed flow fields and convection, at simulated reduced gravity, on the characteristics of the morphological instability generated during the solidification of binary alloys. To use these results to develop strategies to gain some control over the quality of the final product of the solidification process. To determine the suitability of such control strategies in future space experiments.

Task Description:

To study, experimentally and numerically, the types of morphological instability that are to be found during the directional solidification of binary alloys. Attempt to control such instabilities by subjecting the solidifying interface to various types of flow field. Assess the usefulness of a reduced gravity in modifying these processes, in order to improve the quality of, and reduce the defects in, manufactured products. Questions of interest include the selection of length scales, the persistence of traveling waves, and of oscillatory instability in the nonlinear regime.

Task Significance:

The basic methods involved in controlling such nonlinear dynamical phenomena are of general value, and the space environment may provide a suitable test bed for examining such ideas over a wider range of the control parameters, and in more realistic geometries, than can be obtained terrestrially. For example, they could be beneficial in the control of the solidification process in a wide range of applications where an imposed flow could modify or suppress the usually deleterious effects of convection.

Progress During FY 1996:

Over the past year, we have continued our computational investigation into the effects on the solidification process by the presence of a Hele-Shaw flow in a crystal melt. In order to accurately represent the variety of linear and nonlinear mechanisms whose interplay governs the growth of the liquid/solid interface, it is mandatory to employ highly accurate computational procedures. Consequently, we have developed a numerical approach that employs a combination of a Fourier spectral method in the periodic direction and a high-order compact finite difference method in the pulling direction. Away from the boundaries, we employ discrete approximations of central kind and sixth order accuracy, whereas near the boundaries one-sided stencils of third order accuracy are used. These compact finite difference discretizations allow the evaluation of spatial derivatives in the pulling direction with high accuracy as well. The calculation is advanced in time by means of a low-storage third order Runge-Kutta scheme. This combination, in conjunction with an analytical conformal mapping procedure, leads to excellent accuracy.

As a first step, we extended the linear stability theory to account for uniform flow parallel to the nominal interface. The results show that this flow results in the migration of the wavy interfacial perturbation and also affects its growth rate. The wave propagation velocity depends on the strength of the imposed flow. Subsequently, we extended the code for nonlinear numerical simulations to the case of flow in the melt. Test simulations with our nonlinear code show excellent agreement with the linear stability results for all cases. Our plan is to extend the simulations to longer times and larger amplitudes, in order to investigate nonlinear effects in the crystal growth process in detail.

Experimentally a number of goals have been attained. In particular the construction of the apparatus has been completed and a number of preliminary tests carried out. From approximately early-September to the end of the reporting period tests with no applied external flow have been undertaken. Here we hoped to characterize the properties of the SCN-alcohol mixture that was carefully prepared and inserted into the test cell. Pulling rates between 4 and 15 $\mu\text{m/s}$ and a temperature gradient of 2 $^{\circ}\text{C/mm}$ have been used. At all speeds the interface first

developed a wavy instability that evolved to deeper cells with approximately a 150 μm wavelength, which grew at a rate less than the pulling speed (V). Eventually a few cells dominated the growth and a dendritic structure with a wavelength of about 600 μm evolved. These grew at a rate equal to V , but at an angle to the pulling direction that depended on the magnitude of V .

This effect has not been seen before as far as we are aware and we are presently trying to determine its cause. Is it due to some imperfection in the apparatus or is it inherent to the system itself? To this end the interferometric system, that is an integral part of the apparatus, will be used to look at the temperature distribution across the cell to be sure that it is symmetric. Also an array of thermocouples will be used to cross-check the correctness of this determination. Particles will be placed in the cell to see if convective activity is causing this effect, even in such a narrow gap (1 mm). Finally, other binary mixtures will be used to determine if this change has an effect on the phenomenon.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 2

TASK INITIATION: 10/96 EXPIRATION: 9/99

PROJECT IDENTIFICATION: 962-21-07

NASA CONTRACT NO.: NAG8-124

RESPONSIBLE CENTER: MSFC

The Interactive Dynamics of Convection, Flow and Directional Solidification

PRINCIPAL INVESTIGATOR: Prof. Tony Maxworthy

University of Southern California

CO-INVESTIGATORS:

Muntz, E.P.

University of Southern California

Task Objective:

In order to assess and control the effects of residual spacecraft accelerations on the growth of high quality crystals, full numerical simulations will be conducted. It is anticipated that this approach will lead not only to a minimization of the adverse effects of the flow on the crystal growth process, but also to the development of strategies for employing externally imposed flow fields to gain some degree of control over the solidification dynamics. Questions of interest concern the selection of length scales, the persistence of traveling waves, and of oscillatory instabilities in the nonlinear regime. Time dependent direct numerical simulations performed will allow investigation of these mechanisms in isolation, as well as with their combined effects.

Task Description:

1. Study the types of morphological instability that are to be found during the directional solidification of binary mixtures;
2. Attempt the control of such instabilities using forced flow over the solidifying interface and assess the usefulness of reduced gravity in modifying the process, thereby improving the quality and reducing the defect in manufactured products.

Task Significance:

The basic mechanisms involved in controlling such nonlinear dynamical phenomena are of value to other fields of science and engineering, and the space environment may provide a suitable test bed for examining such ideas. This could be beneficial to control the solidification process by employing externally imposed flow fields to improve the quality and reduce defects in manufactured alloy products.

Progress During FY 1996:

As of January 1996 the design and construction of the basic apparatus has been completed. This includes a cell-traversing subsystem, that was not part of the original proposal, but that was found necessary to incorporate the test-cell with the Leitz Interferometric Microscope made available by the Materials Research Section of NASA LeRC. Also, a visit by Dr. Eli Raz was arranged in order to become familiar with the operation and idiosyncrasies of the microscope as quickly as possible. This visit proved to be particularly effective in pointing out a number of problem areas that were then addressed in a subsequent redesign. Also, during this period the acquisition of a supply of 99.999% pure SCN became a source of difficulty. The only known source, Professor M. Glicksman, has a huge backlog of orders. Because of this strong demand and the long time-scale of the production method, we believe that this source cannot be relied upon to supply the needed material in a consistent and timely fashion. Two solutions have been proposed. The first is to build our own zone-refining system based on a commercially available device. However, presently funds are not available to do this. The second solution is to use commercially available SCN (99.9% pure) and use this as the base, "pure" material against which the effect of adding the second component, acetone, can be compared. Experimentation on the techniques needed to fill the cell and to operate the heating and cooling, and especially, the flow-control systems was begun in early January 1996. Up until the end of this task in June 1996, we have run a number of experiments with no flow. The resulting patterns of cells and dendrites make it clear that impurities in the system were causing problems. Upon disassembling the apparatus, it was found that a reaction between the SCM and the brass valves had taken place. The equipment is being rebuilt using stainless steel parts in contact with the SCM.

We have been fortunate in securing independent, one year funding for a student to work on this project. His experience in this area of research has proved invaluable in modifying the original design to include a number of refinements that will improve the overall operation of the system. He is presently supported by a new grant from the NASA Microgravity Program.

Independently, we have also begun work on an interesting fluid dynamical analog to the problem of directional solidification. This steady state version of the so-called "Printer's Instability" is easier to work with experimentally and it is possible to test many of the features of the prototype problem with relative ease. In particular, the problem of the dependence of the instability wave length on the operating parameters, especially the cell gap-width, can be studied in depth and used to interpret the solidification experiments.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/94 EXPIRATION: 6/96**PROJECT IDENTIFICATION: 962-25-05-26****NASA CONTRACT No.: NAG3-162****RESPONSIBLE CENTER: LERC**

Y₂BaCuO₅ Segregation in YBa₂Cu₃O_{7-x} During Melt Texturing

PRINCIPAL INVESTIGATOR: Dr. Paul J. McGinn

University of Notre Dame

CO-INVESTIGATORS:No Co-I's Assigned to this Task

Task Objective:

The objective of this ground-based investigation is to understand the segregation of fine second phase Y₂BaCuO₅ (211) precipitates during so-called "melt texture growth" of the superconductor YBa₂Cu₃O_x (123).

Task Description:

In melt texturing of 123, one of the goals is to refine the 211 that is present in the textured microstructure as much as possible to enhance flux pinning. However, segregation of fine 211 will affect the ability of the 123 to pin magnetic flux. It is unclear if segregation is an unavoidable consequence of precipitates being pushed by the solidification growth front, and what role is played by gravitational effects. The goal of this project is to understand the causes of 211 segregation. The effect of a number of factors on texturing will be examined to determine what is causing the observed segregation.

Through a series of melt texture growth experiments the effect of Pt additions on 211 size, and more importantly the 211 size dependence of segregation, will be determined. The effect of 123 growth morphology on 211 segregation will also be examined. This will allow for determination of whether the observed segregation is specific to only one morphology of 123 growth, or is characteristic of all 123 growth. The growth mode will be altered by using different techniques to achieve 211 refinement. It is anticipated that containerless processing experiments will be included in this part of the study as they will provide the best opportunity to observe impurity-free growth.

After the effect of the above factors is understood experiments will be performed to attempt melt texturing of 123 in a microgravity environment.

Task Significance:

It is expected that this research will identify important factors affecting the segregation of fine 211 particles during the melt texturing of the 123-type high temperature superconductors. It will enhance the understanding of the crystal growth process and the development of the microstructure. It is anticipated that knowledge gained from working with this technologically important system will be applicable to other systems exhibiting similar crystal growth features.

Progress During FY 1996:

In melt texture grown YBa₂Cu₃O_{7-x} (123) "domain" microstructures, often unreacted Y₂BaCuO₅ (211) particles are observed to be present in the form of distinguishable patterns in the form of "tracks." These tracks originate due to interactions between the particles and the solidification front. Our previous work has described a model for the formation of these patterns in individual domains. We have more recently been investigating particle pushing by zone melting to verify if it occurs in zone melted wires (previously not observed) and to attempt to discern the critical growth velocity in this system. In the past year we have demonstrated that particle segregation can be observed in zone melt textured Y-123 with Pt additions. Similar to what is observed during melt texture growth, as the 211 particles become more refined they are able to be pushed by the solidification front. The Y-123 growth front is faceted, with the leading edge typically lying toward the center of the rod. 211 particles are observed to be pushed outward toward the rod periphery by the propagating front, leaving a 211 poor region in the center of the rod.

As the sample speed is changed from 0.5 $\pm$ 0.7 $\pm$ 0.9 mm/hr no change in the extent of 211 segregation is discernible. However, at higher speeds the planar solidification front begins to break down. As the amount of 211 is increased, the size of the 211 depleted region diminishes in area, and the "211 poor region" contains a higher volume of 211. The critical growth velocity appears to be in the same range where the planar growth front breaks

down. As a result, it is difficult to distinguish a distinct critical growth velocity where a stable planar front can be maintained, yet avoid particle pushing. The behavior in rods appears to mimic the behavior we have previously described for crystals grown by melt texture growth. There, sheets of 211 form from being pushed to the edge of the growing crystal. Here they are pushed to the edge of the wire, and simply accumulate to give the observed pattern of radial segregation.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	1	BS Degrees:	1
MS Students:	1	MS Degrees:	1
PhD Students:	0	PhD Degrees:	0

TASK INITIATION: 6/94 **EXPIRATION:** 6/96**PROJECT IDENTIFICATION:** 962-21-08-29**NASA CONTRACT NO.:** NAG8-106**RESPONSIBLE CENTER:** MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Varanasi, C., Black, M.A., and McGinn, P.J. The Demonstration of Y_2BaCuO_3 Particle Segregation in Melt Processed $YBa_2Cu_3O_{7-x}$ Through a Computer Visualization Model. J. Materials Research, vol. 11, 565-571 (1996).

Presentations

Balwada, H., and McGinn, P. " Y_2BaCuO_3 Particle Segregation in Zone Melt Textured $YBa_2Cu_3O_{7-x}$." MISCON Group Meeting, Univ. of Notre Dame, Notre Dame, Indiana, August 1996.

Interaction of Hele-Shaw Flows with Directional Solidification: Numerical Investigation of the Nonlinear Dynamical Interplay and Control Strategies

PRINCIPAL INVESTIGATOR: Prof. Eckart H. Meiburg

University of Southern California

CO-INVESTIGATORS:

Maxworthy, T.

University of Southern California

Task Objective:

In order to assess and control the effects of residual spacecraft accelerations on the growth of high quality crystals, full numerical simulations will be conducted. It is anticipated that this approach will lead not only to a minimization of the adverse effects of the flow on the crystal growth process, but also to the development of strategies for employing externally imposed flow fields to gain some degree of control over the solidification dynamics. Questions of interest concern the selection of length scales, the persistence of traveling waves, and of oscillatory instabilities in the nonlinear regime. Time dependent direct numerical simulations performed will allow investigation of these mechanisms in isolation, as well as with their combined effects.

Task Description:

1. Study the types of morphological instability that are to be found during the directional solidification of binary mixtures;
2. Attempt the control of such instabilities using forced flow over the solidifying interface and assess the usefulness of reduced gravity in modifying the process, thereby improving the quality and reducing the defect in manufactured products.

Task Significance:

The basic mechanisms involved in controlling such nonlinear dynamical phenomena are of value to other fields of science and engineering, and the space environment may provide a suitable test bed for examining such ideas. This could be beneficial to control the solidification process by employing externally imposed flow fields to improve the quality and reduce defects in manufactured alloy products.

Progress During FY 1996:

The presence of flow in a crystal melt generally has an adverse effect on the growth of high quality crystals. In order to minimize the flow, it has hence become popular to conduct solidification experiments in the narrow gap between two parallel flat plates, also known as the Hele-Shaw configuration. However, while the effect of the flow is reduced significantly in this way, it cannot be eliminated completely. Some of the mechanisms for the presence of residual flow are buoyancy-driven convection due to thermal and concentration gradients, as well as volumetric expansion or contraction as a result of concentration changes. We hence have to develop a more complete understanding of the flow's dynamical interplay with the growing crystal, so that strategies can be developed for how to limit its negative side effects and, if possible, for how to obtain some benefits by artificially imposing a controlled flow field. Within the present project, we attempt to advance the understanding of the relevant phenomena through carefully conducted high-quality theoretical and numerical investigations.

In order to accurately represent the variety of linear and nonlinear mechanisms whose interplay governs the growth of the liquid/solid interface, it is mandatory to employ highly accurate computational procedures. Consequently, we have developed over the last 18 months a numerical approach that employs a combination of a Fourier spectral method in the periodic direction and a high-order compact finite difference method in the pulling direction. Away from the boundaries, we employ discrete approximations of central kind and sixth order accuracy, whereas near the boundaries one-sided stencils of third order accuracy are used. These compact finite difference discretizations allow the evaluation of spatial derivatives in the pulling direction with high accuracy as well. The calculation is advanced in time by means of a low-storage third order Runge-Kutta scheme. This combination, in conjunction with an analytical conformal mapping procedure, leads to excellent accuracy.

As a first step, we have extended the linear stability theory to account for uniform flow parallel to the nominal interface. The results show that this flow results in the migration of the wavy interfacial perturbation. The wave propagation velocity depends on the strength of the imposed flow. Subsequently, we extended the code for nonlinear numerical simulations to the case of flow in the melt. Test simulations with our nonlinear code show excellent agreement with the linear stability results for all cases. Our plan is to extend the simulations to longer times and larger amplitudes, in order to investigate nonlinear effects in the crystal growth process.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/94 EXPIRATION: 6/96**PROJECT IDENTIFICATION: 962-25-05-27****NASA CONTRACT NO.: NAG3-161****RESPONSIBLE CENTER: LeRC**

The Synergistic Effect of Ceramic Materials Synthesis Using Vapor-Enhanced Reactive Sintering Under Microgravity Conditions

PRINCIPAL INVESTIGATOR: Prof. John J. Moore

Colorado School of Mines

CO-INVESTIGATORS:

Ready, D.

Colorado School of Mines

Task Objective:

The primary objective of this research is to develop a technique for processing advanced ceramics in the form of fine powders, whiskers or platelets. The secondary objective is to determine the extent of vapor phase reactions, including convection, in combination with gravity driven flow, in the process. Important concerns include product particle size and purity. Products should have particle sizes allowing efficient handling and subsequent processing and/or function. Control of the chemical reactions and particle sized is necessary for the achievement of this objective.

Task Description:

Titanium diboride is synthesized according to the reaction $\text{Ti} + 2\text{B} = \text{TiB}_2$ and titanium diboride + alumina (Al_2O_3) composites are synthesized by the reaction $3\text{TiO}_2 + 3\text{B}_2\text{O}_3 + 10\text{Al} = 3\text{TiB}_2 + 5\text{Al}_2\text{O}_3$. The first reaction was chosen for its relatively simple liquid-solid reaction, allowing the fundamentals of the reaction to be accurately evaluated. The TiB_2 is formed via a combustion synthesis reaction in the propagating mode, which has high product purity and rapid reaction rates as inherent advantages of this process. The second reaction also uses the propagating mode, but is complicated by the fact that the reacting components become both molten and gaseous during the ignition process. Convection, therefore, plays a much greater role than in the first reaction. Both reactions will be carried out in both inert, i.e., Ar gas, and reactive, i.e., HCl gas, environments in order to evaluate the effects of vapor transport on the combustion synthesis reaction. A complete examination of the process variables, including micro and increased gravity, will be completed to examine the effect on the reaction.

The project has taken on two new areas of interest during the FY 1995. The first area is the effect of varying amounts of liquid of varying specific gravity at the reaction front. Reactions will be investigated to achieve liquids with differing specific gravity and quantity at the reaction front. The effect of gravity on density-driven fluid flow will be an important variable in investigating the role of liquid at the reaction front. The first set of experiments will have a range of compositions between TaB_2 and TiB_2 to obtain an increasing amount of liquid at the reaction front.

The second area of interest is the development of a numerical model of the heat transfer processes that take place in a $\text{Ti} + 2\text{B} = \text{TiB}_2$ combustion synthesis reaction. This model should predict the effects of microgravity on the heat transfer process, especially convection.

Task Significance:

Fine powders may be used as raw materials for subsequent processing techniques, while platelets and whiskers may be used as reinforcement materials in composite structures. Evaluation of reactions in microgravity enhance basic understanding of ground-based reaction mechanisms.

Progress During FY 1996:

The recent progress in this final year of the research program has been in two main areas:

1. The effect of gravity on the combustion synthesis of a specific ceramic composite system (i.e., Ti-Ta-B), in which there is a complete range of solid solution of $\text{TiB}_2/\text{TaB}_2$. This system generates different amounts of liquid titanium at, and ahead of, the reaction front as the rates of $\text{TiB}_2/\text{TaB}_2$ changes. Experiments conducted on the NASA LeRC DC-9 aircraft were able to provide data at gravity levels lower than and greater than Earth gravity. The experiments performed in low gravity provided higher combustion temperatures and less segregation in the product microstructures than those conducted at 1g and 2g, where the effects of gravity-driven fluid flow can be significant.

2. The establishment of an accurate temperature/time data collection and analysis system for SHS reactions. This system is built around a Pentium PC.

The graduate student on this program has recently completed his MS thesis defense and is now employed in industry.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	1
PhD Students:	3	PhD Degrees:	0

TASK INITIATION: 1/93 **EXPIRATION:** 12/96**PROJECT IDENTIFICATION:** 962-26-05-10**NASA CONTRACT No.:** NCC3-289**RESPONSIBLE CENTER:** LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Guzman, J.A., Moore, J.J., and Readey, D.W., "Effects of liquid metals during combustion synthesis in the Ti-Ta-B system." American Ceramic Society, Annual Meeting, Indianapolis, April 14-17, 1996.

Lantz, C., Teft, P., Moore, J.J., and Readey, D.W., "Self propagating reactive synthesis of ceramics in a microgravity environments." TMS Symposium "Experimental Methods for Microgravity Materials Science", Eds: R. Schiffman, C. Patielli, pub. by TMS, pp. 41-44, October 1995.

Diffusion, Viscosity, and Crystal Growth in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Allan S. Myerson

Polytechnic University, New York

CO-INVESTIGATORS:

Izmailov, A.

Polytechnic University, New York

Task Objective:

The results of this research should improve the operation and data analysis of existing microgravity crystal growth experiments and aid in the design of new hardware for such experiments.

Task Description:

Components of this research include:

- Experimental studies of the diffusion coefficients and viscosity of triglycine sulfate (TGS), KDP, and other compounds of interest to microgravity crystal growth in supersaturated solutions as a function of solution concentrations, solution age, and solution history;
- Development of a theoretical model of diffusion and viscosity in the metastable state;
- Development of a model of crystal growth from solution including nonlinear time-dependent diffusion and viscosity effects;
- Employment of the model with and without buoyancy-driven convective flows to predict results of Earth and microgravity crystal growth experiments and to compare these results with experimental results; and
- Development of a computer simulation of the crystal growth process that will allow simulation of microgravity crystal growth, including the effects mentioned above.

Plans are to develop the adequate physical description of the crystal growth process in the supersaturated solutions. To achieve this goal, it will be necessary to take into account the nontrivial dependencies of such transport coefficients as diffusivity and viscosity on the solute concentration and solution temperature and age. The research program's approach will include obtaining the characteristic time for the crystal growth process in the supersaturated solutions, i.e., to obtain the duration of the metastable state relaxation that leads the system "crystal + supersaturated solution" to the equilibrium state. This equilibrium is the equilibrium between the crystal surface and the entire remaining volume of the surrounding saturated solution.

Another facet of the program will theoretically determine from the proposed model the difference in the concentration, temperature, and convective flow fields between an Earth-grown crystal and one grown in microgravity. This will also allow a comparison of the gains in face size and stability that might accompany microgravity crystal growth.

Comparison of theoretical predictions to the real experimental data will verify the theoretical model and determine numerical values for model parameters that have not been measured.

Task Significance:

Since crystallization from solution occurs in supersaturated solutions, the properties of these solutions and their role in nucleation and crystal growth are of interest. Recognition of this has led to a number of studies of supersaturated solutions and their properties.

Progress During FY 1996:

Diffusion coefficient of TGS has been measured at several temperatures in the concentrated supersaturated regions.

A method to calculate the degree of association and the number average cluster size of ADP, KDP, and TGS from

activity data in the supersaturate region was developed and is based on the assumption of the clusters being in the form of electrically neutral Bjerrum pairs and their aggregates.

Gradient column experiments to examine clustering in TGC, KDP, and ADP were conducted.

Analysis of concentration profiles around growing crystals accounting for the effect of concentration dependent diffusion coefficient and viscosities was continued.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 3/93 EXPIRATION: 3/96

PROJECT IDENTIFICATION: 962-26-08-09

NASA CONTRACT No.: NAG8-960

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Izmailov, A.F., and Myerson, A.S. Gravity Induced Formation of Concentration Gradients in Supersaturated Binary Solutions. *Physica*, vol. A 244, 503 (1996).

Izmailov, A.F., Myerson, A.S., and Na, H.S. Supersaturated Electrolyte Solutions: Theory and Experiment. *Phys. Rev. E*, vol. 52, 3923 (1995).

Proceedings

Kessel, A.R., Temnikov, A.N., Izmailov, A.F., and Myerson, A.S. "New and Effective Technique to study Supersaturated Solutions by the Pulsed (Spin-Echo) NMR Method." *Crystal Growth of Organic Materials*, ACS, Washington, D.C., p 266 (1996).

Myerson, A.S., and Izmailov, A.F. "Study of Organic Supersaturated Solution: Theory and Experiment." *Crystal Growth of Organic Materials*, ACS, Washington, D.C., p 222 (1996).

Presentations

Izmailov, A.F., and Myerson, A.S. "Moment and Mass Transfer in Supersaturated Solutions and Its Consequences for Crystal Growth from Solutions." *The Tenth American Conference on Crystal Growth*, Vail, Colorado (1996).

Izmailov, A.F., Myerson, A.S., and Na, H.S. "Supersaturated Electrolyte Solutions: Theory and Experiment." *American Institute of Chemical Engineers (AIChE) Annual Meeting*, Miami, Florida (1995).

Izmailov, A.F., Myerson, A.S., Regel, L.L., and Wilcox, W.R. "Influence of High Gravity on Cluster Formation and Nucleation." *The Third International Workshop on Materials Processing at High Gravity*, Clarkson University, New York (1996).

Izmailov, A.F., Myerson, A.S., Regel, L.L., and Wilcox, W.R. "Influence of High Gravity on Cluster Formation and Nucleation." *46th International Astronautical Federation Congress*, Oslo, Norway (1995).

Myerson, A.S., and Izmailov, A.F. "Thermodynamic Properties of Supersaturated Electrolyte Solutions." *The 13th Symposium on Industrial Crystallization*, Toulouse, France (1996).

Myerson, A.S., and Izmailov, A.F. "Fluctuation-Dissipation Theorem for Supersaturated Electrolyte Solutions." *The Tenth American Conference on Crystal Growth*, Vail, Colorado (1996).

An Electrochemical Method to Measure Diffusivity in Liquid Metals

PRINCIPAL INVESTIGATOR: Prof. Ranga Narayanan

University of Florida

CO-INVESTIGATORS:

Anderson, T.
Fripp, A.L.University of Florida
NASA Langley Research Center (LaRC)

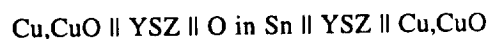
Task Objective:

This research program uses coulometric titration of a solid electrolyte electrochemical cell to measure oxygen diffusivity in liquid metals. Central to this program is an estimation of the effect of low gravity on the measurement of diffusivity. This will lead to the design of experiments where the use of a low gravity environment significantly reduces the adverse effects of convection in the melt. The availability of these "benchmark" values of diffusivity will be useful for assessing the reliability of different experimental designs and operational procedures for measuring diffusivity on earth.

Another science objective of this study is to establish the constitutive behavior of "Fickian diffusion" of oxygen in liquid metals. In particular, we will accurately measure the temperature dependence of the oxygen diffusion coefficient.

Task Description:

In this study an existing experimental "cell" that has been modified by these investigators is used. An example of a system that is studied is the diffusion of oxygen in tin. The experimental arrangement consists of two electrochemical cells sharing a common working electrode, viz: tin. A representation of the cell is given by:



Yttria stabilized zirconia (YSZ) is the solid state electrolyte through which oxygen ions are transported into or out of the liquid tin. In these experiments, one cell is used to establish a known boundary condition, usually a negligibly small oxygen concentration, while the second cell is operated in the open circuit mode to measure the oxygen concentration at the opposite boundary. The solid state electrolytes and tin are physically arranged so that the gravity vector is co-linear with the gradient of concentration.

One of the YSZ disks is at the top and has a small overflow port to accommodate the expansion of tin upon heating. Care is taken to avoid leakage of oxygen from this or other sources. Temperature gradients in this nominally isothermal experiment are reduced to avoid natural convection under earth's gravity. In ground-based experiments it also is important to ensure that oxygen concentration gradients are parallel to the gravity vector so that the melt is not "top heavy." This means that the oxygen concentration should be low at the "bottom" of a vertically oriented cell. This in turn implies that oxygen depletion takes place from the bottom or oxygen addition takes place from the top.

Task Significance:

The availability of a method that gives benchmark values of diffusivity in liquid metals has many uses. These include the assessing of the reliability of different experimental designs and operational procedures for measuring diffusivities under Earth's gravity, as well as defining the constitutive relationships in liquid metals. This latter use is of fundamental importance in understanding the behavior of liquid metals and alloys.

Progress During FY 1996:

This project was successfully completed in December 1995. Electrochemical titrations were performed in two different configurations. In a circular configuration titrations were performed in a steady state mode (i.e., the potential was set at each electrode surface). The measured diffusivities were higher even when the oxygen flux was co-linear with the gravity vector. This was expected because the convection intensity is proportional to the cube of the characteristic length, and in the steady state this is the entire sample height. In another set of experiments the

diffusivity was measured in a rectangular geometry and the measured diffusivities were lower than in the circular geometries. This qualitatively agreed with theory. The ultimate conclusion of this project is that convection does and can corrupt diffusivity measurements and that a microgravity environment will be necessary to obtain a benchmark values of this important thermophysical property. A final report on the project is being prepared for submission to NASA.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	2	BS Degrees:	2
MS Students:	2	MS Degrees:	1
PhD Students:	1	PhD Degrees:	0

TASK INITIATION: 2/93 **EXPIRATION:** 12/95**PROJECT IDENTIFICATION:** 962-25-08-26**NASA CONTRACT No.:** NCC8-20**RESPONSIBLE CENTER:** MSFC

Crystal Growth and Segregation Using the Submerged Heater Method

PRINCIPAL INVESTIGATOR: Dr. Aleksandar G. Ostrogorsky

Rensselaer Polytechnic Institute

CO-INVESTIGATORS:

Müller, G.
Monberg, E.

Universität Erlanger-Nürnberg
AT&T Bell Labs

Task Objective:

Fundamental studies of solute segregation at low levels of melt convection will be conducted using a programmable multi-zone furnace modified for growth by the Submerged Heater Method. The specific objectives of these studies are to:

1. Evaluate the suitability of the multi-zone furnace with the submerged heater to serve as a ground-based solidification facility, useful for pre- and post-flight studies.
2. Seek explanations for previous space experiments not demonstrating the diffusion controlled segregation.
3. Determine the criteria that will allow the diffusion-controlled segregation.
4. Evaluate the benefits of using the SHM within a PMZF for future space experiments.

Task Description:

The research plan is to use the Submerged Heater Method in ground-based experiments for studies of mass transport in the melt at low Ra numbers. The effect of the equilibrium coefficient k will be particularly investigated. The studies will focus on electronics materials previously studied in space (e.g., Ge, InSb) doped with elements having different equilibrium distribution coefficients, ranging from $k \sim 0.5$ to $k \sim 10^{-3}$. Directional Solidification and zone melting procedures will be used during growth. The studies will be conducted using a programmable multi-zone Mellen furnace modified for the SHM. The ground-based experimental and theoretical work will be accompanied by numerical simulations. Numerical simulations will be used to model the transfer processes in the melt and to optimize the growth conditions. Future space experiments designed for the SHM will also be modeled.

Task Significance:

We hope to demonstrate that the multi-zone furnace with the submerged heater is useful for pre- and post-flight studies. The pre-flight studies may help to optimize the future space experiments. Our current "post-flight studies" focus on solvent-solute systems previously used in space (doped Ge, InSb and GaSb). We hope to explain why some space experiments did not result in diffusion controlled segregation.

Progress During FY 1996:

Heat transfer and fluid flow during directional solidification in reduced gravity was modeled using FIDAP and NEKTON. Preliminary results were obtained on three-dimensional convection (with and without the baffle) resulting from residual acceleration acting normally to the ampoule axis. In microgravity, the baffle reduces velocities in the melt by one order of magnitude.

The study of segregation during growth from close-to perfectly stirred melts is completed. Forced convection was generated by rotating and oscillating the submerged heater in the vertical Bridgman configuration. Single crystals were obtained in virtually all experiments. A two-zone transparent furnace was designed and built. The hot zone of the furnace consists of two "Trans Temp" elements (Trans Temp Comp., Chelsea, MA 02150) which offer the advantages of mirror insulation (the growth process can be observed). The stepping motors and data acquisition are computer controlled. Two Ga-doped Ge crystals were grown. One of the two crystals was used as a large (32 mm diameter) single crystal seed for directional solidification in the multi zone Mellen furnace. A silica tube with open ends was used as a crucible.

One GaSb crystals was grown in <111> direction. The polycrystalline charge was synthesized by reacting 6 N purity Ga and Sb in silica ampoules using 58% LiCl - 42% KCl eutectic for encapsulation. A 5.2 mm diameter <111> seed was used. The 32 mm diameter crystal was grown in a silica crucible also under 58% LiCl - 42% KCl encapsulation. The grown crystal was found to have only one single twin and low level of dislocations.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	2	MS Degrees:	2
PhD Students:	1	PhD Degrees:	0

TASK INITIATION: 4/93 EXPIRATION: 11/96

PROJECT IDENTIFICATION: 962-21-08-15

NASA CONTRACT NO.: NAG8-952

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Meyer, S., and Ostrogorsky, A.G. Interface Shape and Segregation in Vertical Bridgman Configuration with and without the Submerged Heater. J. Crystal Growth, (in print).

Meyer, S., and Ostrogorsky, A.G. Forced Convection in Vertical Bridgman Configuration with the Submerged Heater. J. Crystal Growth, (in print).

Presentations

Mayer, S., and Ostrogorsky, A.G. "Forced Convection in Vertical Bridgman Configuration with the Submerged Heater." Tenth American Crystal Growth Conference, Vail, Colorado, August 1996.

Ostrogorsky, A.G. "Solidification by the Submerged Heater Method." Centre d'Etudes Nucleaires in Grenoble, France, May 1996.

Gravitational Effects on the Morphology and Kinetics of Photo-Deposition of Polydiacetylene Films from Monomer Solutions

PRINCIPAL INVESTIGATOR: Dr. Mark S. Paley

Universities Space Research Association (USRA)

CO-INVESTIGATORS:

Antar, B.S.

UTSI (consultant)

Frazier, D.O.

NASA Marshall Space Flight Center (MSFC)

Kim, Y.T.

University of Alabama

Witherow, W.K.

NASA Marshall Space Flight Center (MSFC)

Task Objective:

The objective of this work is to understand how natural convection affects the photo-deposition of polydiacetylene thin films from solution. The effects are manifested in the morphology, microstructure and properties of the films, all of which have a direct impact on the performance of these films for photonic applications.

Task Description:

During photodeposition of polydiacetylene films, UV irradiation of the monomer solution produces thermal density gradients that, under the influence of gravity, cause buoyancy-driven convective flows. Additionally, changes in the chemical composition of the solution result in solutal density gradients that can also lead to convection. Convection affects heat and mass transport to and from the growing film, which, in turn, affect the growth kinetics, and thereby, the morphology, microstructure and properties of the films. One effect that has been observed is the formation of defects in the films which act as light scattering centers and lower the optical quality. These result from precipitation of insoluble polymer in the bulk solution, which gets transported by convection to the surface of the growing film and becomes incorporated, and also, in some cases, from nucleation on the surface of the film itself. The goals of this ground-based research are two-fold: first, determine the extent of convection during photo-deposition of polydiacetylene films from solution, and, second, discern how this convection impacts the growth, nature and properties of the films.

The experimental approach is to monitor both convection in the solution and polymer film deposition at the substrate in hopes of relating the two processes. Convective studies will consist of both numerical modeling of the fluid flows and experimental observation using optical techniques such as interferometry and holography. Film deposition will be monitored in solution using in-situ spectroscopic ellipsometry. Initially, the convection studies and film deposition studies will be conducted separately for practical reasons; however, eventually we hope to be able to perform the two studies simultaneously. We would like to directly observe the formation of defects in the films during the growth process, as well as characterize the films for defects after growth. In addition to studying defect formation in the films, we also intend to determine the effects of convection on the growth kinetics, uniformity and surface roughness of the films, and possibly even on the molecular orientation of the polymer chains.

Task Significance:

Polydiacetylenes are a very promising class of organic polymers for applications in the field of photonics (i.e., using light to process data in a manner analogous to electronics). Advances in the telecommunications industry such as fiber optics, as well as the next generation of supercomputers, require high tech materials such as polydiacetylenes with very specific optical, electronic, and mechanical properties. Devices that capitalize on these properties often require the fabrication of thin films in desired patterns possessing very high optical quality (i.e., good uniformity, minimal defects, and in some cases, appropriate molecular orientation). The formation of such films is not trivial. At MSFC, we have developed a novel process for the formation of polydiacetylene films using photo-deposition from solution with UV light which shows great potential for technological applications. However, on Earth the effects of gravity such as natural convection causes fluid flows which can interfere with the process, causing defects in the films, surface roughness, and even poor molecular orientation. In space we can escape these effects and study film growth under more ideal conditions. The knowledge gained from our research

should then enable us to grow better films on Earth, which, in turn, will enable us to improve upon current photonic devices.

Progress During FY 1996:

Funding for this research commenced in July 1996. Since then our UA co-I's have designed a cell in which photo-deposition can be studied using *in situ* spectroscopic ellipsometry. This cell should also be compatible with convection studies planned in the future. Construction of the cell is underway at UA and is nearly complete. Also, at UTSI preliminary numerical simulations of the fluid flow during photodeposition are being conducted. We are interested in both the fluid flow throughout the entire solution, as well as that in the immediate vicinity of the substrate. These must be treated separately since they occur at very different length scales. At present, the simulations only take into account thermal convection (we believe this is the primary driving force for fluid flow); the film growth kinetics and solutal convection are being ignored. The next step in the fluid dynamic analysis will be to take these into account. Lastly, here at MSFC, we are attempting to outfit a quartz cell with thermocouples in hopes of obtaining experimental thermodynamic data on our system; this will aid in verification of our fluid dynamics calculations.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/96 EXPIRATION: 2/97

PROJECT IDENTIFICATION: 962-21-47

NASA CONTRACT NO.: NCC8-66

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Frazier, D.O., Hung, R.J., Paley, M.S., and Long, Y.T. Effects of Convection During the Photodeposition of Polydiacetylene Thin Films. *J. Crystal Growth*, (1996, accepted).

Paley, M.S., Armstrong, S., Witherow, W.K., and Frazier, D.O. Kinetic Studies on Photodeposition of Polydiacetylene Thin Films from Solution: Preliminary Determination of the Rate Law. *Chem. Mater.*, vol. 8, no. 4, 912 (1996).

Proceedings

Paley, M.S. "Photodeposition of Polydiacetylene Thin Films for Photonic Applications in 1-g and in Microgravity." SPIE Conference, Denver, Colorado, August 1996.

Paley, M.S., and Frazier, D.O. "Photodeposition of Polydiacetylene Thin Films for Photonic Applications in 1-g and in Microgravity." SPIE Proceedings, Denver Colorado, August 1996, vol. 2809, p 114.

Investigation of "Contactless" Crystal Growth by Physical Vapor Transport

PRINCIPAL INVESTIGATOR: Dr. Witold Palosz

Universities Space Research Association (USRA)

CO-INVESTIGATORS:

Gillies, D.

NASA Marshall Space Flight Center (MSFC)

Su, C.-H.

NASA Marshall Space Flight Center (MSFC)

Lowry, S. (Associate)

CFD Research, Inc.

Task Objective:

The primary objective of this study is to evaluate the conditions required for growth of crystals without contact with the side walls by physical vapor transport (PVT) in closed ampoules. The potentials and limitations of this technique ("contactless" PVT - cPVT) with respect to crystal size, growth rate, crystal quality, and the potential benefits of the microgravity environment for this technique will be assessed. The conditions for growth of Pb(Se, Te) by PVT will be determined. The evaluation of capabilities and limitations of the existing facilities and recommendations for space crystal growth facilities with respect to this PVT technique will be made.

Task Description:

1. Development of numerical model of heat and mass transport in the growth system.
2. Development of thermochemical model of transport of Pb(Se, Te) by PVT.
3. Fabrication and/or modification of existing crystal growth furnaces.
4. Experimental investigation of transport of Pb(Se, Te) by PVT.
5. Performing test crystal growth experiments.

Task Significance:

The benefits of the microgravity environment for crystal quality may be offset by strains and related crystal defects caused by interaction of the crystal with the walls of the growth container. The cPVT technique offers improved growth conditions which may be beneficial for crystal growth both under ground and microgravity conditions. The study will provide a comprehensive assessment of the technique as opposed to only limited scope of the literature reports on the subject.

Progress During FY 1996:

1. Development of thermochemical model of mass transport of Pb(Te, Se) by Physical Vapor Transport.
2. Theoretical and experimental study on removal of oxides from electronic materials.
3. Construction of two furnaces with an optical window for monitoring crystal growth processes (80% complete).
4. Construction and testing a new system for measuring residual gases in closed ampoules.
5. Preliminary numerical modeling of the thermal field in the growth ampoules.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/95 EXPIRATION: 12/97

PROJECT IDENTIFICATION: 962-21-08-20

NASA CONTRACT NO.: NCC8-66

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Grasza, K., Trivedi, S.B., Yu, Z., Kutcher, S.W., Palosz, W., and Brost, G.A. "Low supersaturation nucleation and contactless growth of photorefractive ZnTe crystals." ACCG-10/ICVGE-9, Vail, Colorado, August 1996.

Palosz, W. "Removal of oxygen from electronic materials by vapor phase processes." ACCG-10/ICVGE-9, Vail, Colorado, August 1996.

Palosz, W., Gillies, D., Graszka, K., Chung, H., Raghothamachar, B., and Dudley, M. "Characterization of cadmium-zinc telluride crystals grown by "contactless" PVT using synchrotron topography." ACCG-10/ICVGE-9, Vail, Colorado, August 1996.

Investigation of Convective Effects in Crystals Growth by Physical Vapor Transport

PRINCIPAL INVESTIGATOR: Dr. Witold Palosz

Universities Space Research Association (USRA)

CO-INVESTIGATORS:

Volz, M.

Krishnan, A.

Burger, A.

NASA Marshall Space Flight Center (MSFC)

CFD Research Corporation

Fisk University

Task Objective:

The objective of the research is to develop a PVT growth system and to select optimum experimental conditions suitable for a conclusive and meaningful assessment of convection and its effect on the quality of the grown crystals. The system will be used (i) to determine the dependence of convection on fluid dynamic parameters, (ii) to evaluate the effects of the concentration gradient(s) on the c-v interface stability and related morphology of the crystals, and, (iii) to assess practical limitations of the effects of convection on uniformity and interfacial stability of the growing crystals. The research will include a related investigation of a transport of impurities and/or dopants and development and experimental verification of a thermochemical model of mass transport of (Pb, Sn)Te by PVT.

Task Description:

1. Development of numerical model of heat and mass transfer in the growth system.
2. Development of thermochemical model of transport of (Pb, Sn)Te by PVT.
3. Experimental investigation of transport of (Pb, Sn)Te by PVT.
4. Theoretical (numerical modeling) and experimental studies of the conditions required for growing crystals with flat crystal-vapor interface.
5. Theoretical (numerical modeling) and experimental studies of convective flow under different fluid dynamic conditions.
6. Investigation of the effects of convective flow on the quality of the grown crystals.

Task Significance:

The growth conditions and quality of the crystals grown by PVT may be affected by convective phenomena. Thermal and solutal buoyancy forces lead to non-uniform vapor composition and thermal gradients and, thus, to less uniform crystal growth conditions. Generally, steeper composition gradients at the interface (caused by convection) facilitate thermodynamic instabilities of growth and may lead to a downgrade of the quality of the growing crystals. Reduction of convection under microgravity conditions may significantly improve the quality of the grown crystals. The investigation will lead to a growth system suitable for testing the effect(s) of convection on crystal quality in conjunction with experiments performed under microgravity conditions.

Progress During FY 1996:

1. Formulation of the fluid dynamic model for numerical simulations.
2. Calibration of the residual gas measurement system.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-21-20

NASA CONTRACT No.: NAG8-128

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Palosz, W. "Investigation of convective effects in crystal growth by PVT." Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.

Containerless Processing of Composite Materials

PRINCIPAL INVESTIGATOR: Prof. John H. Perepezko

University of Wisconsin, Madison

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The effects of containerless and low gravity processing are investigated in the synthesis of composite materials. Existing models predicting criteria for incorporation of particles dispersed in a melt are applied to metallic systems in a microgravity environment. The specific goals of the proposed research are to determine conditions necessary for an effective dispersion (i.e., uniform distribution of small particles), to characterize the bonding characteristics of particles with the matrix when processed under microgravity conditions, and to determine the implications of the results for effective solidification processing of composites. The ultimate goal of this work is to define conditions necessary for effective containerless or low-gravity processing as well as to determine characteristics which are unique to microgravity processing. Specifically, the results of this work will allow a critical test of existing theoretical models dealing with melt-particle interaction as well as processing conditions for particle incorporation. The outcome of these experiments will also further develop the basic understanding of relationships between microstructure and properties of metal matrix composites during microgravity processing.

Task Description:

The focus of this study is on a model system of pure nickel with a discontinuous dispersion of reinforcement particles. The effects of gravity and containment on the microstructural development in particle reinforced composites is studied using free fall to offset the linear acceleration of gravity. Given the extensive knowledge base of the solidification behavior of nickel, assessment of melt and particle interaction becomes possible through a variety of means. The evaluation of the microstructure obtained during containerless processing allows for understanding of the conditions necessary for a uniform distribution of particles without complications introduced by containing vessels such as chemical contamination or particle/mold interaction. When containerless processing is coupled with solidification during free fall, gravitational effects such as flotation, sedimentation, and density driven convection can be reduced. Variation of the magnetic field allows for vigorous mixing of the particles within the molten matrix, as well as solidification with or without external contact. The degree of undercooling may be controlled by monitoring the temperature with a two-color pyrometer and seeding crystallization with a needle when the desired temperature is reached. Through variation of the amount below the equilibrium freezing temperature a specimen is cooled, the driving force, and therefore the rate of solidification, can be directly influenced. The varied solidification front velocity allows comparison to both predictions made by theoretical models as well as experimental data obtained without containerless or microgravity processing.

Task Significance:

Processing of particle reinforced composites under microgravity conditions can result in more uniform distributions of particles. With the reduction of the effects of gravity, problems inherent to conventional fabrication of metal matrix composites such as flotation, sedimentation, and density-driven convection can be avoided. As has been demonstrated in directional solidification experiments, there is a critical rate at which solidification must occur for full incorporation (i.e., engulfment) of particles to occur. Particle engulfment into a forming solid in directional solidification experiments has been shown to depend on the temperature gradient, the solidification front velocity, and the size of the particles for a fixed chemical composition. The limitation in these experiments has been the container, which changes the shape of the front and which affects distribution of the particles through particle/surface interaction. Solidification under microgravity conditions permits a study of particle distribution without the effects of a container or gravity, which supplements information obtained from prior directional solidification experiments. As with all ground-based microgravity experiments, this work serves as a guideline of steps to be followed in subsequent work actually conducted in space.

Progress During FY 1996:

The central component of the program addressed the use of containerless processing together with an undercooled melt and incorporated particles to develop a critical evaluation of solidification front-particle interactions. Numerous

models for the interaction behavior have been proposed, but critical tests are lacking in many cases due to confounding gravitational effects. A common concept in the interaction models is the critical velocity for particle incorporation. The research plan included a novel experimental design based upon an undercooled melt with particles to distinguish particle incorporation effectiveness as a function of interface velocity in the presence of a distribution of particle sizes. The experimental strategy has allowed for an assessment of various models and governing conditions that have been proposed for particle incorporation.

Model systems of nickel with discontinuous reinforcement particles of aluminum oxide or titanium carbide were studied with containerless processing to isolate effects caused by the forces of gravity and of the containing crucible. Experiments have shown undercoolings of 20-30 K for Ni/TiC, with apparent uniform particle incorporation into the melt. Microstructural analysis showed a transition zone from higher to lower particle density around shrinkage cavities or edges of the sample (i.e., near the point of final solidification of the sample). These results appear to demonstrate the transition from particle incorporation to particle pushing, perhaps caused by a decrease of solidification front velocity. Results also suggest a critical velocity below which particle engulfment is unfavorable. Evaluation of the microstructure and the time required to complete solidification provided estimates of this critical velocity. Further study has identified the copper-aluminum oxide system; the aluminum oxide particles do not appear to act as potent nucleant sites for copper, thus allowing for undercooling to be used effectively as a tool for controlling the rate of solidification.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 0

TASK INITIATION: 7/94 EXPIRATION: 7/96

PROJECT IDENTIFICATION: 962-25-08-31

NASA CONTRACT NO.: NAG8-106

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Perepezko, J.H. "Analysis of Containerless Processing and Undercooled Solidification Microstructures." Microgravity and Materials Science DWG Meeting, Huntsville, Alabama, June 1996.

Analysis of Containerless Processing and Undercooled Solidification Microstructures

PRINCIPAL INVESTIGATOR: Prof. John H. Perepezko

University of Wisconsin, Madison

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The main research objective is the evaluation and analysis of the undercooling and resultant solidification microstructures in containerless processing of selected alloys. Containerless processing in ground-based drop tubes may simulate the microgravity conditions via solidification of liquid droplets under free fall conditions. The containerless environment removes a major source of impurities and heterogeneous nucleation sites, allowing for a large melt undercooling. This enhanced liquid undercooling exposes alternate solidification pathways and novel microstructure development. Controlling the undercooling level provides some control of the operative solidification pathway and the resultant microstructure. The novel structures that may be produced in a ground-based containerless processing facility preview the wide range of materials processing experiments that may be conducted in a space-based laboratory. The results of the ground-based drop tube study will be used to identify critical experimental variables in microgravity processing, and the analysis may be used to design and predict the science requirements for space experiments.

Task Description:

The proposed program represents a balanced experimental and analysis effort directed toward the investigation of drop tube and levitation containerless processing methods in ground-based studies. The investigation will focus on the understanding and analysis of microstructural evolution during solidification of undercooled melts. The degree of liquid undercooling attainable in a laboratory scale (3 m) drop tube and levitation melting system can be altered through the variation of processing parameters such as alloy composition, melt superheat, sample size and gas environment. The solidification behavior is evaluated through microscopy, thermal analysis and x-ray diffraction in conjunction with calorimetric measurements of falling droplets and a heat flow model of the processing conditions to judge the sample thermal history. One of the main components of the proposed investigation will focus on the control of microstructural evolution in Ni-V and Co-Al alloys through the high undercooling levels provided by containerless processing to provide fundamental new information on the control of nucleation. Another central component of the proposed program addresses the use of containerless processing together with an undercooled melt with incorporated particles to develop a critical evaluation of solidification front-particle interactions.

Task Significance:

The microgravity environment provides new opportunities for the control of solidification processes, and the containerless environment afforded by microgravity conditions avoids crucible-induced sample contamination and allows for large undercooling. By analyzing key containerless processing parameters in a ground-based drop tube study, a carefully designed space flight experiment may be planned. One of the main components of the proposed investigation will focus on the control of microstructural evolution in Ni-V and Co-Al alloys through the high undercooling levels provided by containerless processing to provide fundamental new information on the control of nucleation. This investigation will contribute to the understanding of terrestrial solidification processing and will demonstrate that microgravity materials processing can yield novel microstructures and phases that have not been observed previously with terrestrial processing approaches. Another central component of the proposed program addresses the use of containerless processing together with an undercooled melt with incorporated particles to develop a critical evaluation of solidification front-particle interactions. The experimental strategy will allow for an assessment of various models and proposed governing conditions for particle incorporation. This information will be useful in the development of high-strength composite materials. The outcome of this program will provide a unique background for a space experiment, because never before has it been possible to quantify the solidification kinetics in a manner that can be achieved with the proposed experiments.

Progress During FY 1996:

One of the main components of the investigation focuses on the control of microstructural evolution in Ni-V and Co-Al alloys with containerless processing to provide fundamental new information on the control of nucleation.

High undercooling solidification of Ni-V alloys over a range of compositions has yielded a duplex partitionless structure of fcc and bcc phases. Cross-sectional TEM analysis of the containerlessly processed foil samples has indicated that the fcc and bcc grains exist in a columnar grain structure. Because of the short solidification time available and the vastly different nucleation and growth rates that may be expected for the two different phases, it is difficult to comprehend how this structure may develop over a range of compositions. A heterogeneous nucleation kinetics model for rapidly quenched large (mm size) droplet samples has been developed to describe the competition between fcc and bcc phases. The nucleation analysis indicates that with high undercooling and heterogeneous nucleation, the nucleation rates for the two competing phases are similar over a range of compositions in agreement with the experimental results. Moreover, the growth rates for the two phases are similar in the composition range of interest at high undercooling levels. The kinetics model is undergoing further refinement to include the influence of heat flow on microstructural development.

Analysis of phase selection in the Co-Al system extends the results of the Ni-V system to show the generality of the kinetics approach. High undercooling solidification of Co-Al alloys has also yielded a duplex partitionless structure of fcc and B2 (ordered bcc) phases. Based upon the kinetics analysis of the Ni-V and Co-Al systems, a model has been developed to generalize the analysis to predict the range of duplex nucleation for an arbitrary alloy system. This approach will be useful in the development of maps to predict solidification microstructures during processing of materials in space.

The other central component of the program addresses the use of containerless processing together with an undercooled melt with incorporated particles to develop a critical evaluation of solidification front-particle interactions. Initial results have established a suitable system (Cu-Al₂O₃) that exhibits significant melt undercooling in the presence of particles. Numerous models for the interaction behavior have been proposed, but critical tests are lacking in many cases due to confounding gravitational effects. A novel experimental design based upon an undercooled melt with particles is being used to distinguish particle incorporation effectiveness as a function of interface velocity in the presence of a distribution of particle sizes. The experimental strategy will allow for an assessment of various models and proposed governing conditions for particle incorporation.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 4/96 EXPIRATION: 4/00

PROJECT IDENTIFICATION: 962-21-41

NASA CONTRACT NO.: NAG8-127

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Allen, D.R., and Perepezko, J.H. "Kinetic Competition During Duplex Partitionless Solidification." ASM/TMS Fall Meeting, Cincinnati, October 1996.

Allen, D.R., and Perepezko, J.H. "Kinetic Competition During Duplex Partitionless Solidification (invited seminar)." Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland, August 1996.

Allen, D.R., Gremaud, M., and Perepezko, J.H. "Nucleation Controlled Microstructural Development in Al-Si Alloys." Ninth International Conference on Rapidly Quenched and Metastable Materials, Bratislava, Slovakia, August 1996.

Containerless Processing for Controlled Solidification Microstructures

PRINCIPAL INVESTIGATOR: Prof. John H. Perepezko

University of Wisconsin, Madison

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The main research objective is the evaluation of the undercooling and resultant solidification microstructures in containerless processing including drop tube processing and levitation melting process of selected alloys as an experience base for microgravity experiments.

Task Description:

The degree of liquid undercooling attainable in a laboratory scale (3m) drop tube and levitation melting system can be altered through the variation of processing parameters such as melt superheat, sample size and gas environment. In a given sample, the competitive nucleation and growth kinetics between equilibrium and metastable phases controls microstructural development. The solidification behavior is evaluated through metallography, thermal analysis and x-ray diffraction examination in conjunction with calorimetric measurements of falling droplets and a heat flow model of the processing conditions to judge the sample thermal history.

Task Significance:

In the current program studies, solidification microstructures are being examined in selected Ni and Mn based systems. The specific alloy selection is based on a metastable phase diagram analysis that allows for the identification of unique microstructures and microstructural transitions that may be produced by microgravity containerless processing.

Progress During FY 1996:

One of the main components of the investigation focuses on the control of microstructural evolution in Ni-V and Co-Al alloys with containerless processing to provide fundamental new information on the control of nucleation. High undercooling solidification of Ni-V alloys over a range of compositions has yielded a duplex partitionless structure of fcc and bcc phases. Cross-sectional TEM analysis of the containerlessly processed foil samples has indicated that the fcc and bcc grains exist in a columnar grain structure. Because of the short solidification time available and the vastly different nucleation and growth rates that may be expected for the two different phases, it is difficult to comprehend how this structure may develop over a range of compositions. A heterogeneous nucleation kinetics model for rapidly quenched large (mm size) droplet samples has been developed to describe the competition between fcc and bcc phases. The nucleation analysis indicates that with high undercooling and heterogeneous nucleation, the nucleation rates for the two competing phases are similar over a range of compositions in agreement with the experimental results. Moreover, the growth rates for the two phases are similar in the composition range of interest at high undercooling levels. The kinetics model is undergoing further refinement to include the influence of heat flow on microstructural development.

Analysis of phase selection in the Co-Al system extends the results of the Ni-V system to show the generality of the kinetics approach. High undercooling solidification of Co-Al alloys has also yielded a duplex partitionless structure of fcc and B2 (ordered bcc) phases. Based upon the kinetics analysis of the Ni-V and Co-Al systems, a model has been developed to generalize the analysis to predict the range of duplex nucleation for an arbitrary alloy system. This approach will be useful in the development of maps to predict solidification microstructures during processing of materials in space.

The other central component of the program addresses the use of containerless processing together with an undercooled melt with incorporated particles to develop a critical evaluation of solidification front-particle interactions. Initial results have established a suitable system (Cu-Al₂O₃) that exhibits significant melt undercooling in the presence of particles. Numerous models for the interaction behavior have been proposed, but critical tests are lacking in many cases due to confounding gravitational effects. A novel experimental design based upon an undercooled melt with particles is being used to distinguish particle incorporation effectiveness as a

function of interface velocity in the presence of a distribution of particle sizes. The experimental strategy will allow for an assessment of various models and proposed governing conditions for particle incorporation.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0 BS Degrees: 0
MS Students: 1 MS Degrees: 1
PhD Students: 1 PhD Degrees: 1

TASK INITIATION: 12/91 **EXPIRATION:** 11/95**PROJECT IDENTIFICATION:** 963-25-07-06**RESPONSIBLE CENTER:** JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Gremaud, M., Allen, D.R., M. Rappaz, M., and Perepezko, J.H. The development of nucleation controlled microstructures during laser treatment of Al-Si alloys. *Acta Materialia*, 44, 2669 (1996).

Proceedings

Allen, D.R. and Perepezko, J.H. "Kinetic competition during duplex partitionless solidification in Ni-V alloys." *Thermodynamics and Kinetics of Phase Transformations 398*, Proceedings of the Materials Research Society Symposium, J.S. Im, B. Park, A.L. Greer, and G.B. Stephenson eds., 57 (1996).

Perepezko, J.H. and Allen, D.R. "Kinetic competition in undercooled liquid alloys." *Thermodynamics and Kinetics of Phase Transformations 398*, Proceedings of the Materials Research Society Symposium, J.S. Im, B. Park, A.L. Greer, and G.B. Stephenson eds., 3 (1996).

Presentations

Allen, D.R. and Perepezko, J.H. "Kinetic competition during duplex partitionless solidification." ASM/TMS Fall Meeting, Cincinnati, OH, October, 1996.

Allen, D.R. and Perepezko, J.H. "Kinetic competition during duplex partitionless solidification." Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland, August 1996.

Allen, D.R. and Perepezko, J.H. "Kinetic competition during duplex partitionless solidification in Ni-V alloys." Materials Research Society Fall Meeting, Boston, MA, November, 1995.

Allen, D.R., Gremaud, M. and Perepezko, J.H. "Nucleation controlled microstructural development in Al-Si alloys." Ninth International Conference on Rapidly Quenched and Metastable Materials, Bratislava, Slovakia, August 1996.

Perepezko, J.H. "Analysis of containerless processing and undercooled solidification microstructures ." Microgravity and Materials Science DWG Meeting, Huntsville, AL, June, 1996.

Perepezko, J.H. and Allen, D.R. "Kinetic competition in undercooled liquid alloys." Materials Research Society Fall Meeting, Boston, MA, November, 1995.

Comparison of the Structure and Segregation in Dendritic Alloys Solidified in Terrestrial and Low Gravity Environments

PRINCIPAL INVESTIGATOR: Prof. David R. Poirier

University of Arizona

CO-INVESTIGATORS:

Heinrich, J.C.

University of Arizona

Tewari, S.N.

Cleveland State University

Hellowell, A.

Michigan Technological Institute

Task Objective:

A primary goal of this research is to identify the growth conditions for microgravity experiments delineating the macrosegregation, microsegregation, and microstructure in comparison to the same features in directionally solidified alloys grown on Earth with inevitable thermosolutal convection. Also, the research has been concerned with dendrite fragmentation in the mushy region of a casting, the transport of dendrite fragments out of the mushy region into overlying liquid and the possible survival of such fragments, sufficient to allow them to grow into equiaxed grains.

Task Description:

Growth conditions are being defined by combining mathematical modelling and simulation with terrestrial experiments on binary metallic and model alloys. The investigation is carried forward at three universities, the University of Arizona with D.R. Poirier and J.C. Heinrich, Cleveland State University with S.N. Tewari, and Michigan Technological University with A. Hellowell.

Task Significance:

This research relates directly to almost all casting of metals as almost all practical cast metals are alloys which solidify under conditions of directional heat transfer. Alloys develop microstructures of dendrite primary and secondary arms, with micro- and macrosegregation patterns influenced not only by the basic physical processes of solidification but also by convective currents. To separate out the convective effects, microgravity experiments are necessary. Results of this work will eventually be included in numerical models for casting of alloys and will thereby impact alloys and will thereby impact a major portion of the economy.

Progress During FY 1996:

Hypoeutectic Pb-Sn alloys, with composition ranging from 10 to 58 wt. % Sn, were directionally solidified at rates of 4 to 66 $\mu\text{m}/\text{sec}$ in measured thermal gradients of 67 to 110 K cm^{-1} . This resulted in macrosegregation along the length of the directionally solidified alloys. The extent of macrosegregation increased with increasing tin content, becomes maximum for 33.3 wt. % Sn, and decreased with further increase in the tin content.

To accompany the experiments, numerical simulations were done using the thermal conditions and composition of one of the experimental ingots exhibiting "freckles" (also called "channel segregates"). At 2000 s in the simulation, channels along the vertical surfaces were clearly evident and segregation was extensive, even though the leading part of the mushy zone advanced only 1 cm. For example, the concentration of solute in the remelted channels is as much as 31.5% Sn and, of course, some of the Sn is transported from the mushy zone into the all-liquid zone by the upward flowing plumes. With no convection, the simulation showed essentially no macrosegregation except for an initial portion where solidification was affected in a temperature field with a variable gradient. Computer simulations of the same case solidified in an environment with a gravitational acceleration of 9.8 $10^{-3} \text{ m}/\text{sec}^2$ showed that the convection was almost completely suppressed and resulted in no macrosegregation, except the slight macrosegregation in the initial stage of solidification that results from diffusional transport. A preliminary study of "g-jitter" with single frequencies of 0.1, 1 and 10 Hz in the low gravitational field indicated that the "g-jitter" hardly affected the buoyancy driven convection.

Associated with the channels are convective plumes that emanate upward from the channels. Experimental research has been concerned with the transport of dendrite fragments in these plumes and the possible survival of such fragments that allow to grow into equiaxed grains.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 3 BS Degrees: 1
MS Students: 5 MS Degrees: 2
PhD Students: 2 PhD Degrees: 1

TASK INITIATION: 2/93 EXPIRATION: 7/96

PROJECT IDENTIFICATION: 963-25-05-09

NASA CONTRACT NO.: NAG3-144

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Hansen, G., Hellawell, A., Lu, S.Z., and Steube, R.S., Some consequences of thermo-solutal convection: The grain structure of castings. Metall. Mater. Trans. A, vol. 27A, pp. 569- 581 (1996).

Huang, H.-W., Heinrich, J.C., and Poirier, D.R., Numerical anomalies in simulating directional solidification of binary alloys. Numer. Heat Transfer, Part A, (1996).

Huang, H.-W., Heinrich, J.C., and Poirier, D.R., Simulation of directional solidification with steep thermal gradients. Model. Simul. Mater. Sci. Eng., (1996).

Pilling, J., and Hellawell, A., Mechanical deformation of dendrites by fluid flow. Metall. Mater. Trans. A, vol. 27A, pp. 229-232 (1996).

Tewari, S.N., and Shah, R., Macrosegregation during dendritic arrayed growth of hypoeutectic Pb-Sn alloys: Influence of primary arm spacing and mushy zone length. Metall. Mater. Trans. A, (1996).

Proceedings

Hellawell, A., "Grain evolution in conventional and rheo-castings." Proceedings of the 4th Int. Conf. On Semi-Solid Processing of Alloys and Composites, Sheffield, England, pp. 60-65, June 1996.

Presentations

Hellawell, A., "Modelling of casting, welding and advanced solidification processes." Eds. M. Cross and J. Campbell, The Minerals, Metals & Materials Society, Warrendale, PA, pp. 565-584, October 1995.

The Effects of Microgravity on Vapor Phase Sintering

PRINCIPAL INVESTIGATOR: Prof. Dennis W. Readey

Colorado School of Mines

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to develop a better understanding of the effect of gas atmospheres on the sintering of ceramic materials. In a reactive atmosphere, the bonding that occurs between the ceramic powder particles is different than it is in a nonreactive atmosphere. This allows us to control the amount of remaining porosity in the ceramic very precisely. In addition, a reactive atmosphere causes the powder particles to grow much larger and faster than they do in a nonreactive atmosphere. Combining both the controlled bonding and the controlled particle growth, allows us to produce ceramic parts with both controlled amounts of porosity and controlled pore sizes. It is the ability to control the microscopic structure of the ceramics that leads to their interest for filters and composite materials and other applications. Unfortunately, particle growth does not follow the predictions of theory nearly as well as we would like in order to control the process better and to apply it to a wider range of ceramic materials. We believe that one of the reasons for this is that in a ceramic part being sintered, the powder particles are in contact with each other. With other particles surrounding a particle in all directions, it is not able to grow at the rate predicted by theory because of the constraint of these neighboring particles.

However, in microgravity, these powder particle can be dispersed in the gas phase, be completely separated, and not be constrained to grow by neighboring particles. Therefore, we intend to investigate the growth of powder particles dispersed and suspended in a reactive gas in the absence of gravity with the growth of the same powder particles pressed into contact with each other in one-g. From these data, we will be able to determine whether our hypothesis of particles constraining other particles from growing is correct. In addition, we will be able to determine whether the theory for particle growth is correct or whether it needs to be modified for these ceramic materials. Finally, the results of this research will allow us to make improved porous ceramics for a wide variety of applications.

Task Description:

The research task is to use microgravity to develop a better understanding of how atmospheres affect the sintering of ceramics. Most high technology ceramics are made from powders that are heated at high temperatures to increase the chemical bond between the powder particles that results in a hard, temperature and corrosion resistant ceramic material. This process is called "sintering." Understanding how the powder particles bond together during the sintering process and what are the important factors that influence it are extremely important in being able to control and optimize the ceramic fabrication process. For example, one important variable in the sintering process is the gas atmosphere. This research is focused on the effects of the gas atmosphere on the sintering of ceramics. Some atmospheres have little effect. In contrast, however, a reactive atmosphere that reacts with the sintering powder can have a very large effect. We are using such reactive atmospheres in other research to produce new and interesting ceramic materials that cannot be easily made by other methods. For example, with the use of a reactive atmosphere, we are able to control the amount of bonding between the powder particles and can produce porous materials that have many potential applications such as high temperature and corrosion-resistant filters. Another application that we are working on is using these porous ceramics as part of high temperature ceramic-metal composites which are essentially a new class of materials that have a combination of the good properties of both the metal and ceramic.

Task Significance:

The significance of this research is that it will lead to:

1. a better understanding of the sintering of ceramic materials in general;
2. a improved understanding of the effects of gas atmospheres on the sintering of ceramics;

3. new porous ceramic materials that can be used for filters, composites, and many other applications such as radiant burners;
4. the ability to control the sintering of porous ceramics.

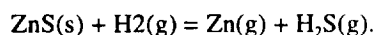
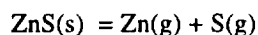
Progress During FY 1996:

This project was funded for only about half of the FY96 fiscal year. Additional funding was to be forthcoming to allow the PhD candidate to finish his work but the funds have yet to appear. In any event, the research continued with various sources of support to allow the PhD candidate to continue his work without his having to change research topics.

Inorganic Surrogate Materials

This work was completed with the completion of the M.S. thesis of James Westhoff. The purpose of these studies was to find a material that would show vapor phase sintering due to its own high vapor pressure or in a reactive atmosphere that was acceptable in a microgravity environment and at low temperatures. In previous studies, HCl has been used as a reactive gas for many systems at elevated temperatures. We were trying to find alternative materials.

It was concluded from these studies that ZnS is an ideal material since it has a high vapor pressure at temperatures at or below 1000 °C that would permit experiments to be carried out with existing shuttle facilities. ZnS undergoes vapor transport by both of the following reactions:



During the last month, we have discovered that CdTe undergoes vapor transport at even lower temperatures. We have been working with Golden Photon, a subsidiary of ACX Technologies, Inc. in Golden, Colorado that makes solar energy systems that use CdS-CdTe solar cells. Working with them, it was determined that vapor phase sintering of CdTe is very important in the processing of their solar cells. A result of this collaboration has been a new patent disclosure on the fabrication of these solar cells that will have far-reaching implications on their commercial viability. Of course, this work was done without NASA funds and will become the property of Golden Photon. If this research project had been continued, it has not, then we would begin work on CdTe since it clearly will satisfy the requirements for an ideal surrogate material for microgravity experiments. In addition, any information that we would gain about the vapor phase sintering of CdTe would greatly benefit Golden Photon's solar cell development as well. However, the work will not continue unless funding from another source can be found.

Organic Surrogates

Over thirty organic compounds were found in the literature that had high vapor pressures at low temperatures. Many were eliminated because of their alleged toxicity and others simply because their melting points were too low or their vapor pressures too high. An example of one such material is H₂O, ice. Although it has many desirable features for this study, handling it below room temperature creates problems that are to be avoided. Cinnamic acid and benzoic acid are reasonable surrogates that show vapor phase sintering behavior at temperatures between 100 °C and 200 °C. However, because of their high vapor pressures, they cannot be observed directly in an electron microscope. As a result, changes in structure had to be followed by making a replica of the structure for microscopic observation. This difficulty plus the fact that these materials are very soft, does not make them good surrogate materials to mimic the behavior of ceramics at high temperatures. The research on the organic surrogates is being completed and incorporated into a second M.S. thesis that will be completed by the end of the calendar year.

Vapor Transport in Multi-Component Systems

In addition to the surrogate materials, another avenue that was to be investigated is the coarsening of more dispersed systems. This is being accomplished in two ways: 1.) investigating coarsening in a multi-component system in

which only one component coarsens; and 2.) investigating coarsening in an extremely low density powder compact made by sol-gel techniques. Work has been initiated with Fe_2O_3 as one of the main constituents in HCl since previous research has shown that this materials is the most well-behaved in terms of coarsening by vapor transport. Also, it coarsens in HCl at temperatures between 900 and 1300 °C so that the existing Crystal Growth Furnace could be used in shuttle experiments. Coarsening experiments have been done in the Fe_2O_3 - Al_2O_3 system which show only limited solid solubility and only the Fe_2O_3 coarsens at low temperatures. The data show that the presence of the Al_2O_3 inhibits the coarsening of the Fe_2O_3 . In contrast, experiments in the Fe_2O_3 -NiO system in which both components coarsen individually under the conditions used, show that coarsening is not inhibited in this system. Conversely, in the NiO- Al_2O_3 system, virtually no coarsening occurs because of the resulting low vapor pressure of AlCl_3 when NiO is also present.

The extremely low density (as low as 10 volume percent solids) powder compacts of Fe_2O_3 to be prepared by sol-gel techniques to investigate coarsening in this lightly constrained system will not be performed because the program was not renewed.

Instead, the focus of the research has now shifted to the fabrication of dense layers of ceramics by vapor phase sintering. The work with Golden Photon and CdTe discussed above has led to the discovery of a very general technique for making both thin and thick layers of virtually any ceramic material. This has important implications for integrated circuits, fuel cells, and thermal barrier coatings. The work has lead to another, more general, patent disclosure at the Colorado School of Mines. Again, since this discovery was made during the period without NASA funding, the patent will be owned by the School.

This research is being performed by the Ph.D. candidate, Darin Aldrich.

Conclusions

The necessity for long flights and non-toxic atmospheres has led to a search for suitable low temperature surrogates to study vapor phase sintering of ceramics. The most promising inorganic compound found to date is ZnS. Although ZnS requires temperatures in the neighborhood of 1000 °C, it has a sufficiently high vapor pressure to produce the desired effects without the presence of a reactive, and possibly toxic, atmosphere. Based on additional research not funded on this project, CdTe may even be a better choice. However, additional work will need to be done to confirms this.

None of the organic surrogates appear to be appropriate.

Research on the multi-component systems confirms the necessity for both species to be volatile in a compound. For example, NiFe_2O_4 exhibits all of the attributes of vapor phase sintering in HCl since volatile chlorides of both iron and nickel are produced at sufficiently high pressure to produce vapor transport. In contrast, with NiAl_2O_4 , vapor phase sintering does not occur due to the low pressure of AlCl_3 in HCl. Also, in multi-component, multi-phase systems such as Fe_2O_3 - Al_2O_3 , the presence of the none-transporting aluminum oxide greatly hinders the vapor phase sintering of iron oxide as predicted.

Future Work

If the additional funds are forthcoming to support the PhD student through the completion of his graduate program, as promised, then the efforts will focus on developing the conditions under which dense layers of ceramics can be formed by vapor phase sintering.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 1

TASK INITIATION: 12/92 EXPIRATION: 12/95

PROJECT IDENTIFICATION: 962-26-05-08

NASA CONTRACT No.: NCC3-289

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

J. C. Westhoff, Model materials for vapor phase sintering in microgravity. M. S. Thesis, Colorado School of Mines, (January, 1996).

Readey, D.W., Aldrich, D.J., and Ritland, M.A., Vapor transport and sintering. Sintering Technology, R.M. German, G.L. Messing, and R.G. Cornwall, eds., (Marcel Dekker, NY), pp. 53-60 (1996).

Readey, D.W. and Ritland, M.A., Reactive vapor phase sintering for the production of porous materials and composites. Processing and Fabrication of Advanced Materials IV, T.S. Srivatsan and J.J. Moore, eds., (TMS, Warrendale, Pa.), pp. 151-164 (1996).

Presentations

Aldrich, D.J., and Readey, D.W., "Vapor phase sintering in multicomponent systems." American Ceramic Society Annual Meeting, Indianapolis, IN, May 1996.

Aldrich, D.J., and Readey, D.W., "Vapor phase sintering of multicomponent ceramics." Poster Presentation at Rocky Mountain Chapter Meeting of the American Vacuum Society, 1st Place Prize in Student Division, 1996.

Aldrich, D.J., Ritland, M. A., and Readey, D.W., "Vapor phase sintering of ceramics." Ceramographic Exhibit, American Ceramic Society Annual Meeting, Indianapolis, IN, 2nd place, SEM category, May 1996.

Readey, D.W., Aldrich, D.J. and Westhoff, J.H., "Vapor phase sintering." Poster Presentation at the NASA Microgravity Materials Science Meeting, Huntsville, AL, June 1996.

Westhoff, J. H., and Readey, D.W., "Model materials for vapor phase sintering in microgravity." American Ceramic Society Annual Meeting, Indianapolis, IN, May 1996.

Modeling of Detached Solidification

PRINCIPAL INVESTIGATOR: Dr. Liya L. Regel

Clarkson University

CO-INVESTIGATORS:

Wilcox, W.R.

Clarkson University

Task Objective:

The long term objective of this research is to develop techniques to achieve detached solidification reliably and reproducibly, in order to produce crystals with fewer defects. To achieve this objective, it is necessary to understand thoroughly the physics of detached solidification. It is the primary objective of the present project to achieve this understanding.

Task Description:

Ingots directionally solidified in space often have had diameters smaller than their containing ampoules, after correcting for the difference in thermal expansion coefficients. It is believed that such ingots have greater crystallographic perfection (i.e., fewer dislocations, twins, and grain boundaries). This is a better reason to grow crystals in space than the classical objective of achieving uniform doping.

Following is our mechanism for detached solidification in space. When solidification first begins, the solid is in intimate contact with the ampoule wall. As it cools from the freezing temperature, stress builds up between the ampoule and the solid because of the difference in their thermal expansion coefficients. Eventually this stress is sufficient to break the solid free from the ampoule. The gap between the solid and the ampoule is filled by evaporation of a volatile constituent from the melt. This constituent, probably residual gas that has dissolved in the melt, had accumulated near the freezing interface because of the usual impurity segregation. The gap width adjusts itself with subsequent solidification until transport of the volatile constituent to the meniscus is sufficient to provide the pressure difference across the meniscus required by surface tension.

The primary FY96 task was to solve the steady state equations under different conditions, to determine the stability of the steady state, and to find out why detached solidification had been observed only in space.

Task Significance:

Solidification in space has often yielded crystals that were smaller in diameter than their containing ampoules. When this occurs, crystals of much higher perfection are produced. We now understand how this occurs and why crystal perfection is greater. This research project aims to put this understanding on a firm basis so that detached solidification can always be achieved. The research should also yield improvements in crystal growth on earth.

Progress During FY 1996:

1. We numerically solved the differential equations governing steady state mass transfer with convection due to solidification and to the variation of surface tension along the meniscus (Marangoni convection). Although Marangoni convection had a strong influence on the local velocity field, it did not strongly affect transport of dissolved gas into the gap or the resulting gap width.
2. We determined the influence of the various physical properties and operating parameters on the steady state gap width. Our emphasis was on the properties of InSb, which has manifested detached solidification in several flight experiments.
3. We determined the stability of steady state detached solidification. The shape of the meniscus is destabilizing, and detached solidification would not be observed without transport of dissolved gas into the gap through the meniscus. This dissolved gas transport is sufficient to stabilize the gap only for a short distance on the order of the gap width. Heat transfer stabilizes the gap up to a distance on the order of the ampoule diameter. This agrees with the results of flight experiments, in which the solid re-attaches to the ampoule wall after a distance on the order of the ampoule diameter.

4. We showed that detached solidification has not been observed on earth because the usual buoyancy-driven convection prevents the build up of rejected volatile species near the freezing interface. On the other hand, we predicted that gentle convection along the freezing interface, from the center toward the ampoule wall, should enhance transport of dissolved gas into the gap and make detached solidification possible on earth. Shortly after this prediction, Dr. Frank Szofran observed detached solidification of germanium in his laboratory at Marshall Space Flight Center, in collaboration with Dr. Klaus Benz of the University of Freiberg.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/94 **EXPIRATION:** 12/96

PROJECT IDENTIFICATION: 962-21-08-21

NASA CONTRACT No.: NAG8-106

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:
Journals

Wilcox, W.R., and Regel, L.L. Detached solidification. Microgravity Science and Technology, vol. 8, 56-61 (1995).

Presentations

Popov, D.I., Regel, L.L., and Wilcox, W.R. "Numerical modeling of detached solidification." American Conference on Crystal Growth - 10, Vail, Colorado (July 1996).

Popov, D.I., Regel, L.L., and Wilcox, W.R. "Numerical Modeling of Detached Solidification." 70th Colloid and Surface Science Symposium, Clarkson University (June 1996).

Regel, L.L., Popov, D.I., and Wilcox, W.R. "Detached solidification: Steady state results." Proceedings of the Microgravity Materials Science Conference, Huntsville, Alabama (June 1996).

Regel, L.L., Popov, D.I., and Wilcox, W.R. "Modeling of detached solidification." IAF Congress, Oslo, Norway (October 1995).

Thermophysical Property Measurement of Molten Semiconductors in 1-g and Reduced-g Conditions

PRINCIPAL INVESTIGATOR: Dr. Won-Kyu Rhim

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Thermophysical properties of molten semiconductors, such as Si, Ge, Si-Ge, and InSb will be measured as a function of temperature using the High Temperature Electrostatic Levitator developed at JPL. Each material will be doped by different kinds of impurities at various doping level. Thermophysical properties that will be measured include:

- density;
- thermal expansion coefficient;
- surface tension;
- viscosity;
- specific heat;
- hemispherical total emissivity; and, perhaps
- electrical conductivity.

Results obtained from the electrostatic levitator will be compared with (or complement) the results obtained by other collaborators both in 1-g as well as in reduced-g environments.

Task Description:

To understand the formation kinetics of a variety of crystal imperfections such as point defects, non-uniform distribution of doping atoms, and other impurity atoms in a growing crystal, the growth process is numerically modeled, inputting various thermophysical properties of molten semiconductors. However, in an environment where accurate thermophysical properties are lacking, crystal growth remains an "art" instead of a "science."

The importance of accurate thermophysical properties of semiconductors in crystal growth cannot be overly emphasized. The total hemispherical emissivity, for instance, has a dramatic impact on the thermal environment. It determines the radiative emission from the surface of the melt, determining to a large extent the profile of the solidified crystal. In order to understand convection and turbulence in the melt, viscosity becomes an important parameter. Surface tension determines the shape of the liquid-atmosphere interface near the solid-liquid-atmosphere triple point. Currently used values for these parameters are very inaccurate, and this program intends to provide more reliable thermophysical properties.

Many molten semiconductors are so reactive with crucibles that dispersed impurities in the melts tend to substantially modify the properties of pure semiconductors. In this program, sample levitation is done in a high vacuum using the High Temperature Electrostatic Levitator which was recently developed at JPL, and thermophysical properties will be measured by applying various non-contact diagnostic techniques. Micro-g experiments will be done by Japanese collaborators using an electromagnetic levitator as the sample is dropped in the 10 second drop-shaft in Hokkaido, Japan. Such comparison studies will help identify those thermophysical properties which are difficult to measure on earth due to the convective flows in the melts, and at the same time, we may be able to identify the most reliable technique which will consistently produce correct values.

Task Significance:

Thermophysical properties of semiconductors both in solid as well as in molten states are needed in order to develop a new crystal growth method for defect free semiconductor crystals. As the dimensions of semiconductor devices continue shrinking, growing more perfect semiconductor crystals became necessary. One crucial step toward this goal is to understand the crystal growth process and the causes of various crystal imperfections such as point defects, non uniform distribution of doping atoms, and impurity atoms in the growing crystals. Such a scientific investigation of semiconductor crystal growth processes requires accurate knowledge of thermophysical properties,

particularly of molten semiconductors. However, accurate thermophysical properties of molten semiconductors are lacking since highly reactive semiconductor melts react with container walls and the true properties are altered. The main objective of this program is to isolate molten semiconductor drops in a high vacuum condition using a recently developed levitation technique, thus maintaining the melts free from container walls as well as surrounding gaseous medium, and to measure their thermophysical properties by applying various non-contact diagnostic methods.

Progress During FY 1996:

The surface tension and the viscosity of a pure silicon have been measured using a transient drop excitation technique developed for the electrostatic levitator (TDET/ESL). In the TDET/ESL, a resonant oscillation is induced by applying a short electric pulse at the near-resonance carrier frequency. The free oscillation following the excitation pulse was observed and analyzed to extract the surface tension and the viscosity. Similar experiments will be repeated until the capability of this technique in 1-g environment is well established.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/96 EXPIRATION: 9/99

PROJECT IDENTIFICATION:

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Rhim, W.-K. "Thermophysical Property Measurement of Molten Semiconductors in 1-g and Reduced-g Conditions (poster presentation)." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Undercooling Limits and Thermophysical Properties in Glass Forming Alloys

PRINCIPAL INVESTIGATOR: Dr. Won-Kyu Rhim

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Spjut, R.E.

Ohsaka, K.

Harvey Mudd College

Jet Propulsion Laboratory (JPL)

Task Objective:

- (i) Investigation of undercooling limits in glass-forming alloys, as those factors that limit undercooling are systematically controlled. Factors that will be examined are sample surface condition, sample volume, cooling rate, material-dependent factors such as viscosity and interfacial energy between solid and liquid, etc.
- (ii) Thermophysical property measurements and investigation of the validity of the classical nucleation theory and other existing theories in the extreme undercooled states. Thermophysical quantities that will be measured as a function of undercooling level are heat capacity, hemispherical total emissivity, surface tension, viscosity, mass density, and thermal expansion coefficient.
- (iii) Investigation of morphological and microstructural development during solidification from deeply undercooled melts. Factors which are investigated through analysis of processed samples are morphology of metastable crystalline or amorphous phase, dependence of microstructure on undercooling level, etc.
- (iv) Evaluation of the limits of electrostatic levitation for containerless materials processing in 1-g environment. This objective will be achieved in collaboration with Prof. William Johnson at the California Institute of Technology and with Prof. Robert Bayuzick at Vanderbilt University. This effort is intended to determine the 1-g limit of the electrostatic levitation technique with respect to achieving their science requirement.
- (v) A feasibility study of a Small Droplet Electrostatic Levitator (SDESL) to change the sample volume by six orders of magnitude. Design and test of several basic technologies such as the electrode assembly, the position detection system, and the sample launch system will be conducted. Reduced funding will not permit the actual construction of a SDESL.

Task Description:

The primary objective of this program is to produce deeply-undercooled metallic liquids and to identify factors which limit undercooling and glass formation. The generally accepted heuristics for achieving deeper undercooling are: increase sample cooling rate, decrease sample volume, isolate the sample from heterogeneous nucleants, increase liquid/solid interfacial energy, and increase the reduced glass-transition temperature or the liquid viscosity. This research is an ambitious attempt to examine these heuristics and to investigate phase transformation in the deeply undercooled liquids in a quantitative manner. That is, analysis of experimentally observed undercooling/nucleation phenomena will be rigorously carried out using classical nucleation theory with the support of experimentally determined thermophysical properties under the same conditions in temperature and pressure. This work will be conducted in collaboration with Professor William Johnson at the California Institute of Technology in his efforts to determine physical properties of undercooled glass forming alloys.

Task Significance:

Some metallic alloys easily turn into glassy states (or amorphous states) having novel physical and chemical properties. For example, a family of glassy metal alloys developed by researchers at Caltech have about three times the strength of steel although the density is 25% lower than steel. The alloys also show low coefficient of friction and excellent corrosion resistance. Utilizing the thermal plasticity of the undercooled viscous state which takes place between the glass transition and solidification temperatures, melts can be injected into molds for net-shape component fabrication. To extend their properties for wide engineering applications more scientific research is required to understand those factors which prevent the alloy melts from glass formation. Such glass formation usually takes place when molten alloys are deeply undercooled well below their usual solidification temperatures.

These undercooled melts are very unstable against contacts with container walls and inclusion of certain foreign materials. It is the purpose of this task to investigate the glass formation processes of various metal alloys in a high vacuum environment while the melts are levitated by the recently developed electrostatic levitator.

Progress During FY 1996:

The first-cut design parameters of a Small Droplet Electrostatic Levitator (SDESL) have been laid out. It includes subsystems such as the drop generation and launch system, the position detection system, the sample charging and heating subsystems, and the temperature measurement system. Each subsystem will be developed independently before they are integrated into the final system. A high power laser (100 watt) for sample heating along with necessary safety system have been installed in a new laboratory which will be dedicated to this project.

STUDENTS FUNDED UNDER RESEARCH:**TASK INITIATION: 7/96 EXPIRATION: 9/99****PROJECT IDENTIFICATION:****RESPONSIBLE CENTER: MSFC**

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Rhim, W.-K. "Undercooling Limits and Thermophysical Properties in Glass Forming Alloys (poster presentation)." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Drop Tube Operation

PRINCIPAL INVESTIGATOR: Dr. Michael B. Robinson

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective is to maintain and upgrade the operation capability of and to conduct experiments in the MSFC 105-meter drop tube. The drop tube facility includes, in addition to the tube itself with the associated pumps and valves, such items as furnaces, levitators, other sample holding or handling devices, and data recording systems. This research includes the operation of a facility laboratory located at the facility. This laboratory includes furnace test facilities as well as pyrometer calibration platforms.

Task Description:

This research covers work in the area of defining, developing, and conducting experiments using the low-gravity capabilities of the drop tube. Such experiments may be in themselves complete investigations to develop new knowledge or to prove theories, or they may serve as precursors for more extensive experiments to be conducted in space. This research also includes studies and experiments to define the effects of various levels and durations of acceleration perturbations on microgravity experiments.

The research approach will be to:

- Study the limits of undercooling in a low-gravity containerless environment and ascertain if nucleation occurs homogeneously at the undercooling limits.
- Evaluate the effects of deep undercooling by containerless processing on resulting microstructure and define and understand the types of phases formed, their shapes and sizes, and their distribution, abundance, composition, homogeneity, and substructure.
- Study the formation of quasi-crystalline material through deep undercooling.
- Study the spreading of liquids as a function of undercooling in order to better understand the thermophysical properties of materials.

Task Significance:

This research activity is an essential part of a successful program of research in microgravity science and applications. Many experiments proposed for flight on the Space Transportation System (STS) can be developed and tested in preliminary form using drop facilities. This can result in significant savings through the proving of experiment concepts and equipment designs before proceeding to much more costly space flight hardware. It also provides additional data that can be compared with data obtained from the space flight experiments. And in some cases, the data obtained from the drop tube or aircraft experiments prove to be sufficient to satisfy the experimenter's requirements, thus obviating the need to proceed with an experiment on the STS. The result is an overall savings in the cost of conducting microgravity experiments while adding to the scope and quality of the results obtained.

Progress During FY 1996:

In the past year, effort has been directed to supporting six flight and ground-based investigations. Approximately 600 research samples and a much larger number of test samples were processed in the Drop Tube in support or preparation for these investigations. The supported investigations and a brief description of the science objectives are listed below:

- Dr. Kenneth F. Kelton, Washington University at St. Louis: A study of the effect of low-gravity, containerless processing on the formation and properties of quasi-crystalline materials.

- Dr. Merton C. Flemings, Massachusetts Institute of Technology: An attempt to measure the viscosity and surface tension of undercooled metals samples by recording the shape and rate of the spreading front from a splat quenched sample.
- Dr. William L. Johnson, California Institute of Technology: A study of the thermophysical properties (heat capacity, surface tension, viscosity) of metallic glass forming materials.
- Dr. Robert J. Bayuzick, Vanderbilt University: A measurement of the distribution of nucleation temperatures of undercooled metals and alloys.
- Dr. Richard N. Grugel, Universities Space Research Associates/NASA MSFC: A study of the effect of undercooling on hypomontectic alloy systems.
- Dr. Michael D. Robinson, NASA Marshall Space Flight Center: A study of the separation and undercooling phoneme in immiscible metal systems through low-gravity, containerless processing.

In addition to supporting the above named research efforts, the Drop Tube facility is actively supporting a study of the effect of welding in space on space suit materials in support of MSFC's Materials and Processing Laboratory.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 1/78 **EXPIRATION:** 1/97

PROJECT IDENTIFICATION: 962-28-08-02

RESPONSIBLE CENTER: MSFC

Measurement of the Optical and Radiative Properties of High-Temperature Liquid Materials by FTIR Spectroscopy

PRINCIPAL INVESTIGATOR: Dr. Michael B. Robinson

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Khrishan, S.

CRI

Rathz, T.

University of Alabama, Huntsville (UAH)

Workman, G.

University of Alabama, Huntsville (UAH)

Task Objective:

The objective is to fully develop the use of FTIR spectroscopy for the purpose of determining, at a high rate of speed, the normal and total hemispherical emissivities of deeply undercooled materials over the wavelength range of 2 to 20 microns. Due to the nature of the approach, the spectral emissivities can be determined quickly over a wide wavelength range and applied over a wide temperature range.

Task Description:

The task will involve development of the technique of measuring the radiative properties of high-temperature, highly reactive materials in the liquid and undercooled liquid state by use of FTIR spectroscopy. The sample will be positioned in a containerless environment by either electromagnetic or electrostatic positioners. The technique offers the advantage of fast measurement so that sample temperature stability will not present insurmountable problems.

Task Significance:

Optical property measurements are essential to the understanding of the behavior of liquids at high temperature. Accurate knowledge of these properties provide an ability to validate theories of nucleation, solidification, and undercooling, and provide the basis for accurate non-contact temperature measurement. They are particularly needed for accurate measurement of high temperatures so that existing and new thermophysical property measurements can be interpreted correctly.

Progress During FY 1996:

Research in the FTIR program over the past year has been in the design and development of the FTIR system and adaptation for the specific purpose of measuring the high temperature optical properties of undercooled metals. A complex innovative optical system has been designed and developed. In addition, a modified electromagnetic levitation system has also been designed and is nearing completion. Immediate plans are to begin measurement of the optical properties of standard samples and blackbodies to be used as calibration sources. Next the research will concentrate on the optical properties of undercooled high-purity elements, such as zirconium and niobium.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/94 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 962-25-08-32

NASA CONTRACT NO.: NAG8-106

RESPONSIBLE CENTER: MSFC

Undercooling Behavior of Immiscible Metal Alloys in the Absence of Crucible Induced Nucleation

PRINCIPAL INVESTIGATOR: Dr. Michael B. Robinson

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Frazier, D.

NASA Marshall Space Flight Center (MSFC)

Facemire, B.

NASA Marshall Space Flight Center (MSFC)

Rathz, T.

University of Alabama, Huntsville (UAH)

Workman, G.

University of Alabama, Huntsville (UAH)

Task Objective:

The objective of this effort is to determine if processing immiscible metals in a containerless environment would alter the critical point wetting mechanism and the extent to which this would lead to changes in the subsequent nucleation kinetics. If the nucleation kinetics are suppressed enough to allow bulk undercooling, the nucleation recalescence will be measured. In addition, the droplet surface conditions can be varied by processing in a vacuum versus a gas environment to alter the surface composition and thereby the wetting potential of the fluid phases.

Task Description:

Research in a containerless, low-gravity environment provides much information as to whether preferential wetting of the free surface occurs and more importantly whether it can be controlled. The MSFC 105 Meter Drop Tube Facility will provide the low-gravity, containerless environment necessary for this study.

Task Significance:

Cooling of monotectic alloys into the miscibility gap will lead to nucleation of droplets within the liquid matrix. Previous earth and space experiments have concentrated on the morphology of the bulk microstructure by attempting to control the convective-diffusive flow of these droplets with the proper selection of the crucible material and thermal fields. Immiscible metal systems have as yet not been studied in a containerless environment, eliminating crucible induced flows.

Progress During FY 1996:

Over the past year effort has been centered on initial studies of a number of immiscible systems. From these initial studies, three representative systems, those of Ni-Cr, Ga-V, and Ti-Ce have been selected for more in-depth study. Initial processing and analysis of samples from these three systems indicate a wide range in the separation behavior after processing. The included figure shows the microstructure of a Ni-Cr alloy compared to a processed Ti-Ce sample showing the difference in homogeneous versus separated structure. In addition there is a range in undercooling behavior depending on sample composition, environment pressure, and amount of overheat. Next year's studies will continue with the intent of concentrating on the selected representative systems.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 9/94 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 962-25-08-33

NASA CONTRACT NO.: H-15269D

RESPONSIBLE CENTER: MSFC

A Study of the Undercooling Behavior of Immiscible Metal Alloys in the Absence of Crucible-Induced Nucleation

PRINCIPAL INVESTIGATOR: Dr. Michael B. Robinson

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Frazier, D.O.

NASA Marshall Space Flight Center (MSFC)

Facemire, B.R.

NASA Marshall Space Flight Center (MSFC)

Rathz, T.J.

University of Alabama, Huntsville (UAH)

Workman, G.L.

University of Alabama, Huntsville (UAH)

Task Objective:

The primary objective of this research will be to study the effect of the low-gravity, containerless processing environment on the wetting and separation phenomena of immiscible metal alloys. Within this framework there are many separate objectives necessary to satisfy the primary objective. These are listed below.

- 1) To understand the effect of processing environment and processing technique on the separation phenomena.
- 2) To understand the effect of critical parameters on the separation phenomena. These parameters include composition, overheating, cooling rate, and relative activity of the individual species.
- 3) To attempt to control the separation process by proper selection of the processing environment and critical parameters.
- 4) Provide comparison of results in metal immiscible systems to continuing research with model organic systems.
- 5) Provide comparison of results to theoretical predictions and provide extension of current separation theory to metal immiscible systems.

A secondary objective will be to include and understand the effect of undercooling on the separation phenomena. Since low-gravity containerless processes are conducive to deep undercooling, this objective is a natural extension of the primary objective.

Task Description:

Since different processing environment, processing techniques, and critical parameters will be compared during the study, it is necessary to study a large matrix of samples. After preliminary investigations to select systems for more intense study, samples from selected systems will be processed in the Low-Gravity environment of the 105 Meter Drop Tube Facility. Samples will be melted, then released and allowed to cool, undercool, and solidify during free-fall. Processing parameters, such as alloy composition, ambient pressure of the gas environment, overheating, and degree of undercooling will be varied and studied. In conjunction studies will be performed for comparison in electromagnetic Levitators and using splat quenching techniques. Results will be compared to current theory.

Task Significance:

Through the study of the separation phenomena in low-gravity (i.e. containerless processing), it is should be possible to gain an understanding of the processing parameters which influence separation in immiscible systems. Through this understanding it is hoped that one could predict and possibly control separation. Finally, one must be able to predict and control separation in order to predictably influence the properties of the final product.

Progress During FY 1996:

After initial testing with a number of immiscible systems as planned, three systems were selected for further detailed study. Future work will center around the Ti-Ce, Ni-Cr, and Ga-V immiscible systems. Initial research and metallurgical analysis has shown that the variety in range of separation necessary for this study can be observed

through these systems. Preliminary results indicate complete separation in the Ti-Ce system with homogeneous dispersions in selected samples of the other two systems. Processing of a wide range of compositions and a study of the undercooling behavior is currently underway.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 **EXPIRATION:** 5/00

PROJECT IDENTIFICATION: 962-21-42

NASA CONTRACT NO.: NAG8-128

RESPONSIBLE CENTER: MSFC

Determination of the Surface Energy of Liquid Crystals from the Shape Anisotropy of Freely Suspended Droplets

PRINCIPAL INVESTIGATOR: Dr. Charles S. Rosenblat

Case Western Reserve University

CO-INVESTIGATORS:

Taylor, P.L.

Case Western Reserve University (CWRU)

Task Objective:

We shall implement a program of ground-based experimental studies of the surface shape of droplets of smectic liquid crystals suspended in an intense magnetic field gradient. The initial goal of this work will be to determine the fundamental properties of these materials by measuring the anisotropy in their surface energy; a related theoretical program will be implemented concomitantly. As a magnetic field introduces certain perturbing effects in the liquid crystal molecular orientation, the ultimate goal will be to determine how best to design flight experiments that can yield the same information when the magnetic field used for levitation is absent.

Task Description:

We intend to investigate surface tension and anchoring effects in liquid crystals by suspending droplets of smectic or nematic material in air and in other immiscible liquids using a large magnetic field gradient. We shall observe shape changes as a function of temperature, droplet size, liquid crystalline phase, and material. The combined experimental/theoretical effort will be aimed at understanding both anchoring - the anisotropic part of the surface tension - and gravitational effects, especially at a free surface. To date the issue of liquid crystal anchoring has been clouded by our inability to produce a clean and well defined surface; a free surface clearly meets this criterion.

Although one can achieve a near zero gravity environment in a magnet-based system, one still must be aware of the need to account for magnetic field effects. As many organic materials, especially liquid crystals, have a significant magnetic susceptibility anisotropy, the magnetic field will tend to orient the liquid crystal within the droplet (especially in the nematic phase) or orient the entire droplet (in the smectic phase). Although these effects may provide important information about defects in liquid crystals, it is important that ultimately a space-based experiment be performed to obviate these spurious effects.

Experiments will be performed at Case Western Reserve University using an 8.2T superconducting magnet with transverse optical access. It will be necessary to insert a pole piece in order to achieve a sufficient magnetic force to cancel gravity. Initially, *in situ* observations will be performed with a boroscope and video imaging system. Ultimately we intend to perform electro-optic measurements within the magnetic field. Additionally, the facilities at the National High Magnetic Field Laboratory in Tallahassee will be used.

Task Significance:

Liquid crystals are elongated organic molecules with many interesting and technologically important physical traits. In addition to their inherent scientific importance, liquid crystals are playing an increasingly important (even dominant) role in the display industry, currently estimated to be \$10B per year. Thus, there is widespread interest in characterizing and understanding many of the fundamental properties of these materials. As all liquid crystals displays are housed between solid substrates, there is much need for precise knowledge of the surface energy of liquid crystalline materials. An ideal way to determine the surface energy would be to measure the surface curvature of a free droplet of the fluid, and hence calculate the anisotropy of surface energy. This is possible only in a microgravity environment. Thus, our measurements will provide not only new scientific insight into these anisotropic fluids, but will play an important role in the burgeoning display industry.

Progress During FY 1996:

The first three months of the project were used for development of experimental techniques. As the droplets will be suspended in an 8.2T superconducting magnet, it was necessary to design appropriate pole pieces to enhance the diamagnetic forces on the droplet in order to overcome gravity. The particular pole piece will depend on the nature of the experiment. For example, a pole piece might be needed to achieve uniformity of force, and another to achieve a rapid spatial variation of the force, especially if we desire to compress the droplets. Other important issues include

radial stability of the droplet and location of the droplet within the magnet (for imaging purposes). To achieve these goals, preliminary calculations of the magnetic field profile were performed with simple pole piece designs. Realizing that it would be necessary to use tapered and partially hollowed pole pieces for specific applications, Dr. Robert Weggel (magnet designer at the Francis Bitter National Magnet Laboratory) was enlisted as a consultant. Very recently several specific designs were returned, which will be machined shortly.

During this period we settled on an appropriate imaging system for observing the droplets in the magnet. Funds were obtained from a third source, and the boroscope and image capturing system were ordered. Delivery is expected before winter.

In addition to suspending droplets in air or vacuum, it is also possible to suspend droplets in water. As many liquid crystals are insoluble in water, we've settled on two: pentylcyanobiphenyl (5CB) and pentyloxycyanobiphenyl (5OCB). The former exhibits an isotropic - nematic - crystalline phase sequence, and the latter has a smectic A phase between the nematic and crystalline phases. Careful density measurements were performed, allowing us to achieve a near neutral buoyancy condition in a mixture of D₂O and H₂O. A much weaker magnetic field is then needed to adjust the total force to achieve neutral buoyancy. Work inside the smaller magnet, a 1.5T electromagnet which does not require specialized pole pieces for the liquid crystal/water experiments, is getting under way.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-21-48

NASA CONTRACT NO.: NAG8-127

RESPONSIBLE CENTER: MSFC

Modeling of Macroscopic/Microscopic Transport & Growth Phenomena in Zeolite Crystal Solutions under Microgravity

PRINCIPAL INVESTIGATOR: Dr. Albert Sacco

Worcester Polytechnic Institute

CO-INVESTIGATORS:

Gatsonis, N.A.

Worcester Polytechnic Institute

Alexandrou, A.

Worcester Polytechnic Institute

Durgin, W.

Worcester Polytechnic Institute

Task Objective:

A theoretical study will be performed of zeolite crystal growth in silica solutions. By using macroscopic fluid dynamics, coupled with first-principles microscopic physics and advanced particle simulations, we will study: (a) the effect of transport phenomena and nutrient flow under microgravity conditions along with (b) the nucleation process and (c) the microscopic crystal growth dynamics.

Task Description:

To develop an understanding of zeolite nucleation and growth.

Task Significance:

To date there is no complete or accepted mechanism for zeolite crystallization. These theoretical results coupled with ground and flight experiments should provide the frame work to understand this complex and industrially important field.

Progress During FY 1996:

The contract started late in FY96 (July 1996). To date we have hired a graduate student to start the macroscopic modeling, have begun the search for a post-doctoral fellow, and wrote and presented one paper.

STUDENTS FUNDED UNDER RESEARCH:**TASK INITIATION:** 7/96 **EXPIRATION:** 6/98**PROJECT IDENTIFICATION:** 962-21-31**NASA CONTRACT NO.:** NAG8-125**RESPONSIBLE CENTER:** MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Presentations**

Alexandrou, A., Gatsonis, N., Durgin, W., and Sacco, Jr., A. "Modeling of Macroscopic/Microscopic Transport Phenomena In Zeolite Crystal Solutions Under Microgravity Conditions." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Undercooling Limits in Molten Semiconductors and Metals: Structure and Superheating Dependencies

PRINCIPAL INVESTIGATOR: Prof. Frank G. Shi

University of California, Irvine

CO-INVESTIGATORS:

Rhim, W.K.
Rulison, A.J.Jet Propulsion Laboratory (JPL)
Space Systems/Loral

Task Objective:

The objective of this work is to study the onset of nucleation of crystals and thus the undercooling limits for melts of semiconductors and metals in order to experimentally test and further develop a model for the onset of nucleation.

Task Description:

To investigate the dependence of the degree of supercooling of metastable melts preceding the onset of solidification on the level of melt overheating above the equilibrium liquidus or melting temperature.

Task Significance:

The importance of the relationship between the degree of supercooling and the level of superheating can be understood, for example, in connection with the soldering operations. A certain degree of overheating is often required in soldering operations for a better wetting of a solder. However, such an overheating can often lead to the supercooling of the solder joints which can consequently be misaligned or disconnected and thus a premature mechanical jolting. The importance can also be understood in connection with an interesting potential for the production of new metastable materials. The onset of nucleation in the supercooling liquids and thus the achievable supercooling level determines the selection of the final microstructures and formation of metastable amorphous phases. The ability to predict and control the onset of nucleation is therefore important in advanced materials processing.

Progress During FY 1996:

The dependence of the degree of supercooling of metastable melts preceding the onset of solidification on the level of melt overheating above the equilibrium liquidus or melting temperature is investigated on Sn, Bi and SnPb. We demonstrate for the first time the dependence of the degree of supercooling on the level of superheating can be either abrupt or continuous. In particular, the dependence is bound by two discontinuous limits, and the linear continuous relationship between the degree of supercooling and the level of superheating as described in textbooks is only one of special possibilities. The observed abrupt and continuous relationships can be tentatively linked to the transient structural evolution of melts during melting and solidification, and are probably general, occurring also for other alloys including SnSb.

STUDENTS FUNDED UNDER RESEARCH:BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 10/94 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 962-21-08-22

NASA CONTRACT No.: NAG8-108

RESPONSIBLE CENTER: MSFC

Gravitational Effect on the Development of Laser Weld-Pool and Solidification Microstructure

PRINCIPAL INVESTIGATOR: Dr. Jogender Singh

Pennsylvania State University

CO-INVESTIGATORS:

Mazumder, J.

University of Illinois at Urbana

Metzbower, E.A.

University of Illinois at Urbana

Marsh, S.

Naval Research Laboratory

Task Objective:

This new program is underway to study the effect of convection and mass transport on the laser weld-pool shape and microstructure under solidification conditions that vary between reduced gravity and 2g. The three major driving forces for convection in laser welding are buoyancy (gravity driven), thermocapillary (surface tension gradient driven) and thermosolutal (concentration gradient driven) flows. In normal earth gravity, thermocapillary flow was found to be the dominant force. The investigation will carry out systematic experimental and theoretical studies to identify the regimes of the various convection forces and their effect on the microstructure and quality of the resulting weldments.

Task Description:

Laser welding is a complex process. It includes convection, surface tension, heat and mass transfer, which have an influence on the microstructure and weld pool shape during solidification. These processes are all dependent directly or indirectly on gravitational forces. For the better understanding of these variables, an integrated research effort will be carried out, including mathematical modeling and laser welding of Single Crystals of Pure Iron, Fe-15%Ni-15%Cr Alloy and NiAl. Microstructure of the laser welded region will be characterized by the analytical high resolution transmission electron microscope (HRTEM). This investigation will allow the determination of the distribution of alloying elements across the interface during solidification under various forces. Such analysis will be used to determine the factors dominating on the melt pool shape under different gravitational forces.

Task Significance:

The significance of these investigations is to advance the basic understanding of weld pool shapes and microstructures as influenced by various forces including surface tension, natural-convection, and diffusion. This knowledge is very important for the laser welding of materials in the space (i.e., microgravity).

Progress During FY 1996:

A micro-macro model of solidification in laser welded material is being developed. A stereology based formalism has been used to simplify the incorporation of microscopic models in a macroscopic numerical simulation. A set of uniform stereological parameters has been used to track the geometric properties of the evolving microstructures. The macroscopic state variables at each finite-element node serve as global constraints on the local unit volume of microstructure, which permits direct coupling within and between the micro and macro regimes. Work is now proceeding on applying this approach to dendritic growth and to coupling of solidification with melt convection. Modeling of the melt pool geometry as a boundary condition for the numerical simulations is currently being performed.

Samples for initial experimental studies have been obtained. Some transmission electron microscope (TEM) and scanning electron microscope (SEM) samples have been prepared. SEM studies have been performed on a sample of a weld done on the KC-135 by Jack Weeks of the NASA Marshall Space Flight Center. This sample was stainless steel 304 and the SEM analysis was performed on a segment of the weld that had been made during the reduced gravity part of the flight. TEM specimens of the same sample have been made. Sample rods of Fe-15%Cr-15%Ni and Fe-18.5%Cr-11.5%Ni alloys have been prepared for a ground laser weld experiment to be performed in November. Pre-weld SEM analysis on these materials is being performed.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 **EXPIRATION:** 5/00

PROJECT IDENTIFICATION: 962-21-43

NASA CONTRACT No.: NAG8-127

RESPONSIBLE CENTER: MSFC

Flight Experiment to Study Double Diffusive Instabilities in Silver-Doped Lead Bromide Crystals

PRINCIPAL INVESTIGATOR: Dr. N. B. Singh

Northrop-Grumman Corporation

CO-INVESTIGATORS:

Balkrishna, V.

Northrop Grumman Corporation

Suhre, D.

Northrop Grumman Corporation

Duval, W.M.B.

NASA Lewis Research Center (LeRC)

Coriell, S.

National Institute of Standards and Technology (NIST)

Task Objective:

The objectives of the present programs are to:

- Observe and study the double diffusive and morphological instabilities in controlled conditions and compare with theoretically predicted convective and morphological instability curves.
- Study the three dimensional morphological instabilities and resulting cellular growth that occur near the onset of morphological instability in the bulk samples under purely diffusive conditions.
- Understand the micro- and macro-segregation of silver dopant in lead bromide crystals in microgravity.
- Determine the inter-diffusion coefficient of AgBr and PbBr₂ in the molten state by analyzing the concentration distribution of silver in the lead bromide crystal grown in LEO and compare with theoretically determined values.
- Significantly reduce acoustic and optical scattering in doped lead bromide crystal caused by convection for AO applications.
- Provide basic data on convective behavior in alloy crystals grown by the commercially important Bridgman crystal growth process.

Task Description:

This research program will provide a quantitative understanding of convective effects and a comparison of data with predictions will be carried out using dynamical stability theories developed for thermo-solutal (double diffusive) convection. The purification of as-received (typically 99+% purity) high purity PbBr₂ source material will be carried out by directional solidification followed by zone-melting, and final purity will be evaluated by emission spectroscopy and spark source mass spectroscopy. The transparent space-qualified furnace will be adapted and operated for the ground-based experimentation at Northrop Grumman using Bridgman growth; each thermal zone will be independently controlled during the run.

The ground-based experiments in the space furnace configuration will be carried out with two ampoules doped with silver doped PbBr₂. During these ground-based experiments, convective and morphological instabilities will be observed for different growth conditions in 1-g conditions using a vertical orientation. A detailed analysis will be carried out to calculate the convective and morphological stability curve for the PbBr₂ - AgBr system. Experimental observations obtained from the ground-based experiments in the space furnace configuration will be used to develop and test the validity of a theoretical stability curve for 1-g and micro-g conditions.

Micro- and macro- segregation characterization studies will be carried out on the crystals grown in terrestrial and microgravity conditions at fixed thermal gradient and velocity. The results will be evaluated to examine the effect of convection on the segregation behavior. This result will provide critical information on the difference in segregation patterns compared to pure diffusion-controlled growth. Crystal homogeneity/optical quality will be examined by studying optical transparency, scattering and birefringency interferometry, X-ray rocking curve, X-ray contour scans as well as sample microstructure and microchemistry, and the results will be used to provide characterization of the sample.

Preparation for the space-based experiment in LEO will be carried out by preparing the Science Requirements Document based on the findings of our experiments. We plan to grow PbBr₂ crystals doped with AgBr in LEO in the transparent furnace. Real-time observations on the solid-liquid interface will be taken during the flight in different conditions and results will be compared with theory. The as-grown crystal will be analyzed for segregation after the flight.

The terrestrial studies can be summarized as follows:

Purification of Lead Bromide - The directional freezing technique will be used to initially purify as-received lead bromide. The zone-refining technique will be used to further purify the materials to their required level of 5-9's. Samples will be analyzed to verify achievement of the 5-9's purity.

Design of Convection Cell and Temperature Measurements - Experiments will be carried out in the Bridgman crystal growth geometry. Ampoules will be heated in a cylindrical two-zone furnace. The ampoule design will be modified to meet the specification of the space furnace. The temperature distribution in the solid and liquid will be measured by inserting fine thermocouples in the ampoule during solidification.

Test of Stability Theory - Experiments will be carried out to observe the convective and interfacial instabilities and the results will be compared with the theoretically predicted stability diagram.

Characterization - The morphology of the solidification front will be observed directly at low as well as high magnification to study any interface changes which evolve during crystal growth. Present experiments on lead bromide will also provide information on convective and interfacial stability. The optical transparency of the earth-grown and space-grown crystals will be compared, and the spatial distribution of optical scattering in the crystal will be mapped by a laser beam method for earth grown and space grown crystals. Crystal quality will be examined using x-ray rocking curves, x-ray contours, etchpit techniques and a specialized birefringence interferometry method to examine the effect of fluid flow on optical homogeneity. Microprobe measurements will be selectively employed to characterize the chemical homogeneity of the samples.

Task Significance:

It is nearly impossible to study three-dimensional interface instabilities in bulk samples on earth under purely diffusive growth conditions. The present program on microgravity experiments on transparent lead bromide/silver bromide alloys would enable study of various three-dimensional morphologies that develop near the onset of morphological instability. Crystal growth of lead bromide doped with various concentration of silver bromide at different growth velocities in low earth orbit will allow direct observation of three-dimensional instability and resulting cellular growth. A quantitative examination and comparison of these observations with theoretical morphological and convective stability calculations is not available. The present study will provide the boundary lines to design the crystal growth experiments with reduced convection. The improved homogeneity in a crystal can be achieved if a completely diffusion controlled growth conditions are maintained in the system during growth. The gravitational forces produce perturbations on earth in the nutrient supply and heat distribution that adversely affect the crystal homogeneity. These perturbations are due to gravity driven buoyant convection. The solutal (density difference between silver bromide and lead bromide) and thermal convection can be reduced by six order of magnitude in low earth orbit. In the case of lead bromide, where thermal conductivity of liquid is approximately 1.6 times that of solid, it is not possible to completely avoid the radial temperature gradient. In microgravity we expect to have almost complete elimination of transverse temperature gradient induce incomplete mixing of silver bromide in lead bromide to provide better control of lateral compositional distribution in the melts and stresses resulting from hydrostatic pressure.

Progress During FY 1996:

A two zone transparent glass furnace was calibrated for directional freezing of as supplied lead bromide material. The temperature gradient for this furnace was 31 K/cm. We are using a pull rate of 2 cm/day for purification. The crystal growth furnace was calibrated by using a lead bromide probe. A thermal gradient of 20 K/cm was observed for this furnace. We are carrying out a test experiment to determine the time of development of double diffusive instability at different growth rate. For this experiment we are using a growth ampoule filled with 5000 ppm AgBr doped lead bromide. As supplied lead bromide was listed for 99.999% pure. Further purification was carried out by a combination of directional freezing and zone-melting techniques. The purified material was filled in a 13x15 mm

diameter ampoule with a square seed holder. The seed was oriented in <110> orientation and fabricated to fit in the growth tube.

The change in the shape of solid-liquid interface during crystal growth was observed to be dependent on growth velocity, AgBr concentration and temperature gradient. We are carrying out a test experiment with an ampoule containing 5000 ppm impurity. The temperature gradient is 20 K/cm near the interface. The main objective of this experiment is to determine the time required for the development of instability. We observed that at smaller growth velocity it took a very long time to develop the instability.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 7/96 EXPIRATION: 7/00

PROJECT IDENTIFICATION: 962-21-21

NASA CONTRACT No.: NAS8-408

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Singh, N.B., Mani, S.S., Adam, J.D., Coriell, S.R., Glicksman, M.E., Duval, W.M.B., Santoro, G.J., and DeWitt, R. Direct Observations of Instabilities. *J. Crystal Growth*, vol. 166, 364 (1996).

Proceedings

Mani, S.S., Singh, N.B., Coriell, S.R., Glicksman, M.E., and Duval, W.M.B. "In situ Observations of interface instability During Growth of Lead Bromide Crystals." *Proceedings of "Materials Research Society, Optoelectronic Materials, Ordering Composition, Modules and self Assembled Structures"* (E.D. Jones, A. Mascarenhas, and P. Petroff, eds.) vol. 417, 381-386 (1995).

Presentations

Singh, N.B. "Assessing the Crystal Growth and Operating Characteristics of Acousto-Optical Materials." Anna University, Madras, India, January 28-30, 1996.

Singh, N.B., Coriell, S.R., Mani, S.S., Glicksman, M.E., and Duval, W.M.B. "Flight Experiment to Study Double Diffusive Instabilities in Silver doped Lead Bromide Crystals." *Microgravity Materials Science Conference*, Huntsville, Alabama, June 10-12, 1996.

Double Diffusive Convection during Growth of Lead Bromide Crystals

PRINCIPAL INVESTIGATOR: Dr. N. B. Singh

Westinghouse Electric Corporation

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The main objective of this program is to evaluate, understand and eliminate thermosolutal convection during the crystal growth of $\text{PbBr}_2\text{-AgBr}$ systems. The program will provide a quantitative understanding of convective effects and a correlation of experimental data with theories developed for thermosolutal convection will be carried out. For the $\text{PbBr}_2\text{-AgBr}$ system less dense solute causes the convective (thermosolutal) instability in addition to morphological instability. Also, this system is optically transparent and we can monitor the interface shape to study the convective and morphological instabilities. The technical objectives of this program are to define the parameter at normal gravity to minimize the thermosolutal convection during growth of doped lead bromide crystals to achieve homogeneous distribution of dopant, significantly reduce the optical and acoustic scattering caused by convection during lead bromide crystal growth, and produce lead bromide crystals with unparalleled optical homogeneity for advanced device applications. This will be achieved by experimentally verified stability diagrams and direct observations of solid-liquid interface during crystal growth.

Task Description:

To achieve these objectives, crystal growth experiments will be conducted on earth and in space. Measurements involving Rayleigh number as a function of aspect ratio, and the radius of the growth tube to the length of the melt column, will be made. Experimental results will be compared with the stability diagram to test the validity of morphological and convective stability theories.

Task Significance:

The scientific objectives of this program are to understand the thermosolutal convection during the crystal growth of $\text{PbBr}_2\text{-AgBr}$ system. This will be achieved by growing five crystals at five different concentrations, which will lead to different solutal convective levels. The experimental values of the concentration distribution will be compared with the theories based on pure diffusional growth to evaluate the effect of convection. Also, numerical studies will be carried out to study the convective and morphological instabilities, and to determine the critical concentration of dopant for a particular growth velocity and gravity level. Theoretical instability diagrams will be compared with the experimental studies. Relevant analytical characterization techniques are to be used to evaluate the effect of convection on crystal quality. These studies will provide basic data on convective behavior in doped lead bromide crystals grown by the commercially important Bridgman process.

Progress During FY 1996:

We observed and studied the double diffusive and morphological instabilities in controlled conditions during growth of doped lead bromide crystals. We determined the diffusion coefficient of silver bromide in the liquid lead bromide by using a membrane diffusion method of McBain and Dawson. The experimental value was $1.71 \pm 0.065 \times 10^{-5} \text{ cm}^2/\text{s}$. The ratio of thermal conductivities was determined by measuring the temperature of solid and liquid in the steady state conditions. The liquid thermal conductivity was determined to be $10.26 \times 10^{-4} \text{ Cal/K.s.cm}$, a value 1.65 times higher than that reported for the solid. A detailed study on the effect of convection on crystal quality was carried out by growing lead bromide crystals in transparent Bridgman furnace. Direct observations were taken on solid-liquid interface and a new kind of instability was observed. This could be explained on the basis of toroidal flow in the AgBr -doped lead bromide sample.

The technical objectives of this study was to define the material and processing parameters at normal Earth gravity to minimize the deteriorious effects of thermosolutal convection during growth of doped lead bromide crystals to achieve homogeneous distribution of dopant. Achieving crystal growth with significantly reduced optical and acoustic scattering caused by convection may lead to the availability of lead bromide with unparalleled optical homogeneity for advanced device applications.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/93 EXPIRATION: 9/94

PROJECT IDENTIFICATION: 962-24-05-01

NASA CONTRACT No.: NAS3-258

RESPONSIBLE CENTER: LeRC

Kinetics of Nucleation and Growth from Undercooled Melts

PRINCIPAL INVESTIGATOR: Prof. Frans A. Spaepen

Harvard University

CO-INVESTIGATORS:

Aziz, M.J.
Turnbull, D.

Harvard University

Harvard University

Task Objective:

The objective is to develop a basic understanding of the phenomena and processes that are central to the microgravity program: crystal nucleation and growth, glass formation, the structure and thermodynamics of the crystal-melt interface, and diffusion in the liquid state.

Task Description:

Crystal nucleation is studied in elemental metal, semiconductor, or quasi-crystal-forming droplets coated with different fluxes, droplets with clean surfaces in vacuum, and droplets solidified in a drop tube. Glass formation in metallic systems is studied by fluxing and drop tube techniques. The crystal-melt interfacial tension is studied experimentally and theoretically. A parameter-free test of the theory for dendritic growth is being conducted, and the conditions for oscillatory instabilities are being explored. The diffusivity in the liquid state is measured from the broadening of impurity profiles after pulsed laser melting.

Task Significance:

Studies of the undercooling of liquids and the kinetics of crystal nucleation are an important category of experiments that exploit the containerless environment provided by microgravity. Our work, ground-based, is aimed at advancing the understanding of the fundamentals of undercooling, nucleation, and glass formation; at exploring the potential and limitations of ground-based alternatives such as fluxing and drop-tube processing; and at exploring the potential of ground-based containerless processing facilities provided by the microgravity program.

Progress During FY 1996:

The work on the undercooling of liquid elemental semiconductors has continued. Development of a new $\text{SiO}_2\text{-BaO-CaO}$ flux, with the necessary fluidity and chemical compatibility to be used with molten Si, allowed us to get undercoolings of up to 350K. Comparison of these nucleation data with those obtained by Stifler *et al.* on laser-melted Si films led to the determination of a positive temperature coefficient of the crystal-melt interfacial tension. The interfacial model developed to account for this temperature dependence was also applied to the undercooling of liquid Ge. More recent data on the undercooling of Si, obtained by Herlach's group (DLR), indicate an even higher temperature coefficient. Analysis of the interfacial structure implied by the new observations requires a change in the interfacial thickness. The analysis indicates that a new series of laser-melting experiments should be carried out, in which the new techniques for time-resolved temperature measurements, developed in our laboratory, are used to narrow the uncertainty on the undercooling temperatures under these conditions. These experiments are currently being designed.

To explore the possibility of undercooling bulk liquid Ni into the glassy state (plausible based on an analysis of the temperature dependence of its volume), we have carried out a series of experiments in the Pd-Ni-P system. It is well known that $\text{Pd}_{40}\text{Ni}_{40}\text{P}_{20}$ is an easy glass former that can be made into cm-size samples. We have explored several compositions in the direction of Ni on the ternary composition diagram. It was found that alloys; up to 60% Ni could be made at least partially glassy at cooling rates around 1 K/s. More Ni-rich alloys were always crystalline. An investigation of Ni-rich quaternary and quinary alloys is under way.

We have made considerable progress in the analysis of crystal nucleation in a drop falling in a gas atmosphere within a drop tube. Earlier work had led to a full picture of the evolution of the temperature in the drop, as well as the fluid flow induced by the shear at the surface. Recently we have added the analysis of crystal nucleation. Nuclei are introduced by Poisson statistics, based on steady-stated classical nucleation theory. Their growth is heat flow limited. The evolution of nucleus populations has been studied as a function of the crystal-melt interfacial tension.

Populations containing as many as d30 nuclei have been created. The aim is to apply the results to experimental data we obtained earlier on the nucleation of the Laves phase $MgZn_2$ from a Ga-Mg-Zn melt. The analysis indicates that the interfacial tension is indeed low, as expected from the nature of the structural discontinuity in this system. Work is continuing on increasing the nucleus concentrations and in the incorporation of transient effects.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/96 EXPIRATION: 4/00

PROJECT IDENTIFICATION: 962-21-44

NASA CONTRACT NO.: NAG8-125

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Isono, N., Smith, Patrick Michael, Turnbull, D., and Aziz, M.J. Anomalous diffusion of Fe in liquid Al measured by the pulsed laser technique. *Metallurgical and Materials Transactions A*, vol. 27, 725-730 (1996).

Shao, Y., and Spaepen, F. Undercooling of bulk liquid silicon in an oxide flux. *J. of Applied Physics*, vol. 79, 2981-2985 (1996).

Proceedings

Spaepen, F., and Shao, Y. "The crystal-melt interface in Si or Ge." *Materials Research Society Symposium Proceedings*, 398, 39-44 (1996).

Presentations

Aziz, M.J. "Pressure- and stressed-enhanced kinetics." *International Conference on Diffusion in Materials*, Nordkirchen, Germany, August 1996.

Aziz, M.J. "Rapid solidification." *Advanced Technology Research Laboratories*, Nippon Steel, Kawasaki, Japan, March 1996.

Aziz, M.J. "Rapid solidification." *Central Research Laboratories*, Kobe Steel, Kobe, Japan, March 1996.

Aziz, M.J. "Rapid solidification." *Central Research Laboratories*, Matsushita Electric Industrial Company, Kyoto, Japan, March 1996.

Aziz, M.J. "Research opportunities in highly nonequilibrium growth by pulsed laser deposition." *Institute of Materials Science*, University of Tsukuba, Tsukuba, Japan, March 1996.

Aziz, M.J. "Fundamental issues in nonequilibrium growth by pulsed laser deposition." *Research Laboratory of Engineering Materials*, Tokyo Institute of Technology, Yokohama, Japan, March 1996.

Aziz, M.J. "Experimental constraints on nonequilibrium interface kinetic models." *Ninth International Conference on Rapidly Quenched and Metastable Materials*, Bratislava, Slovakia, August 1996.

Spaepen, F. "Measurements of Interface Stress and Interfacial Enthalpy." *Materials Research Society Fall Meeting, Symposium on Metastable Metal-Based Phases and Microstructures*, Boston, Massachusetts, November 1995.

Spaepen, F. "The Temperature Dependence of the Crystal-Melt Interfacial Tension." *Materials Research Society Fall Meeting, Symposium on Thermodynamics and Kinetics of Phase Transformations*, Boston, Massachusetts, November 1995.

Spaepen, F. "Kinetics of Nucleation and Growth From Undercooled Melts." *Microgravity Materials Science Conference*, Huntsville, Alabama, June 1996.

Spaepen, F. "The interface between a crystal and its melt: Structure, tension, and implications for nucleation." *Materials Science Colloquium*, University of Virginia, Charlottesville, Virginia, October 1995.

Spaepen, F. "The interface between a crystal and its melt: structure, tension, and implications for nucleation." *Department of Mechanical Engineering*, Yale University, New Haven, Connecticut, February 1996.

Spaepen, F. "Structure and thermodynamics of interfaces." DeVivio Lecture in Materials Science, Northeastern University, Boston, Massachusetts, March 1996.

Spaepen, F. "Effect of structural non-uniformity on the temperature dependence of the crystal-melt interfacial tension." Ninth International Conference on Rapidly Quenched and Metastable Materials, Bratislava, Slovakia, August 1996.

Spaepen, F. (Key Invitee and Rapporteur) "Evolution of Film Microstructure and Morphology." ARPA/NSF Workshop on Modeling of Film Growth and Deposition Processes, Institute for Mathematics and Its Applications, University of Minnesota, Minneapolis, Minnesota, January 1996.

Crystal Nucleation, Hydrostatic Tension, & Diffusion in Metal and Semiconductor Melts

PRINCIPAL INVESTIGATOR: Prof. Frans A. Spaepen

Harvard University

CO-INVESTIGATORS:

Aziz, M.J.

Harvard University

Turnbull, D.

Harvard University

Task Objective:

The objective is to develop basic understanding of the phenomena and processes that are central to the microgravity program: crystal nucleating, glass formation, and diffusion in the liquid state.

Task Description:

Crystal nucleation is studied in elemental metal, semiconductor, or quasi-crystal-forming droplets coated with different fluxes, droplets with clean surfaces in vacuum, and droplets solidified in a drop tube. The effect of hydrostatic stress on the nucleation kinetics is studied by dilatometry. The crystal-melt interfacial tension is studied experimentally and theoretically. The diffusivity in the liquid state is measured from the broadening of impurity profiles after pulsed laser melting.

Task Significance:

Studies of the undercooling of liquids and the kinetics of crystal nucleation are an important category of experiments that exploit the containerless environment provided by microgravity. Our work, ground-based, is aimed at advancing the understanding of the fundamentals of undercooling, nucleation, and glass formation; at exploring the potential and limitations of ground based alternatives such as fluxing and drop-tube processing; and at exploring the potential of ground-based containerless processing facilities provided by the microgravity program.

Progress During FY 1996:

The work on the undercooling of liquid elemental semiconductors has continued. Development of a new $\text{SiO}_2\text{-BaO-CaO}$ flux, with the necessary fluidity and chemical compatibility to be used with molten Si, allowed us to get undercoolings of up to 350K. Comparison of these nucleation data with those obtained by Stiffler et al. on laser-melted Si films led to the determination of a positive temperature coefficient of the crystal-melt interfacial tension. The interfacial model developed to account for this temperature dependence was also applied to the undercooling of liquid Ge. More recent data on the undercooling of Si, obtained by Herlach's group (DLR), indicate an even higher temperature coefficient. Analysis of the interfacial structure implied by the new observations requires a change in the interfacial thickness.

To explore the possibility of undercooling bulk liquid Ni into the glassy state (plausible based on an analysis of the temperature dependence of its volume), we have carried out a series of experiments in the Pd-Ni-P system. It is well known that $\text{Pd}_{40}\text{Ni}_{40}\text{P}_{20}$ is an easy glass former that can be made into cm-size samples. We have explored several compositions in the direction of Ni on the ternary composition diagram. It was found that alloys; up to 60% Ni could be made at least partially glassy at cooling rates around 1K/s. More Ni-rich alloys were always crystalline. An investigation of Ni-rich quaternary and quinary alloys is under way.

We have made considerable progress in the analysis of crystal nucleation in a drop falling in a gas atmosphere in a drop tube. Earlier work had led to a full picture of the evolution of the temperature in the drop, as well as the fluid flow induced by the shear at the surface. Recently we have added the analysis of crystal nucleation. Nuclei are introduced by Poisson statistics, based on steady-stated classical nucleation theory. Their growth is heat flow limited. The evolution of nucleus populations has been studied as a function of the crystal-melt interfacial tension. Populations containing as many as 30 nuclei have been created. The aim is to apply the results to experimental data we obtained earlier on the nucleation of the Laves phase MgZn_2 from a Ga-Mg-Zn melt. The analysis indicates that the interfacial tension is indeed low, as expected from the nature of the structural discontinuity in this system.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 4/92 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 962-25-07-07

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Isono, N., Smith, Patrick Michael, Turnbull, D., and Aziz, M.J. Anomalous diffusion of Fe in liquid Al measured by the pulsed laser technique. Metallurgical and Materials Transactions A, 27, 725-730 (1996).

Shao, Y. and Spaepen, F. Undercooling of bulk liquid silicon in an oxide flux. Journal of Applied Physics, 79, 2981-2985 (1996).

Proceedings

Spaepen, F. and Shao, Y. "The crystal-melt interface in Si or Ge." Materials Research Society Symposium Proceedings, 398, 39-44 (1996).

Presentations

Aziz, M.J. "Pressure- and stressed-enhanced kinetics. International Conference on Diffusion in Materials." Nordkirchen, Germany, August 1996.

Aziz, M.J. "Rapid solidification." Advanced Technology Research Laboratories, Nippon Steel, Kawasaki, Japan, March 1996.

Aziz, M.J. "Rapid solidification." Central Research Laboratories, Kobe Steel, Kobe, Japan, March 1996.

Aziz, M.J. "Rapid solidification." Central Research Laboratories, Matsushita Electric Industrial Company, Kyoto, Japan, March 1996.

Aziz, M.J. "Research opportunities in highly nonequilibrium growth by pulsed laser deposition." Institute of Materials Science, University of Tsukuba, Tsukuba, Japan, March 1996.

Aziz, M.J. "Research opportunities in highly nonequilibrium growth by pulsed laser deposition." Institute of Materials Science, University of Tsukuba, Tsukuba, Japan, March 1996.

Aziz, M.J. "Fundamental issues in nonequilibrium growth by pulsed laser deposition." Research Laboratory of Engineering Materials, Tokyo Institute of Technology, Yokohama, Japan, March 1996.

Aziz, M.J. "Experimental constraints on nonequilibrium interface kinetic models." Ninth International Conference on Rapidly Quenched and Metastable Materials, Bratislava, Slovakia, August 1996.

Spaepen, F. "Measurements of interface stress and interfacial enthalpy." Materials Research Society Fall Meeting, Symposium on Metastable Metal-Based Phases and Microstructures, Boston, Massachusetts, November 1995.

Spaepen, F. "The temperature dependence of the crystal-melt interfacial tension." Symposium on Thermodynamics and Kinetics of Phase Transformations, Boston, MA, November, 1995.

Spaepen, F. "Key Invitee and Rapporteur." ARPA/NSF Workshop on Modeling of Film Growth and Deposition Processes Q Evolution of Film Microstructure and Morphology, Institute for Mathematics and Its Applications, University of Minnesota, Minneapolis, Minnesota, January 1996.

Spaepen, F. "Kinetics of nucleation and growth from undercooled melts." Microgravity Materials Science Conference, Marshall Space Flight Center, Huntsville, Alabama, June 1996.

Spaepen, F. "The interface between a crystal and its melt: Structure, tension, and implications for nucleation." Materials Science Colloquium, University of Virginia, Charlottesville, Virginia, October 1995.

Spaepen, F. "The interface between a crystal and its melt: structure, tension, and implications for nucleation."
Department of Mechanical Engineering, Yale University, New Haven, Connecticut, February 1996.

Spaepen, F. "Effect of structural non-uniformity on the temperature dependence of the crystal-melt interfacial tension."
Ninth International Conference on Rapidly Quenched and Metastable Materials, Bratislava, Slovakia, August 1996.

Micro- and Macro-Segregation in Alloys Solidifying with Equiaxed Morphology

PRINCIPAL INVESTIGATOR: Dr. Doru M. Stefanescu

University of Alabama, Tuscaloosa

CO-INVESTIGATORS:

Nastac, L.

University of Alabama, Tuscaloosa

Curreri, P.

NASA Marshall Space Flight Center (MSFC)

Leon-Torres, J.

University of Alabama, Tuscaloosa

Task Objective:

The objective of this research is to develop a model for macro/microsegregation applicable to cast alloys. The new model should include the influence of: (i) buoyancy-driven flow (thermosolutal convection); (ii) convection caused by the relative motion of the liquid/solid interface; and, (iii) convection caused by density variation with change of phase, on both micro- and macrosegregation. The analysis will be conducted for both equiaxed dendritic and eutectic alloys, and columnar dendritic alloys.

Microgravity experimentation will be used to assess the relative value of the three factors affecting solute redistribution. The experimental work will be performed on the DC-9 aircraft for multidirectional solidification, on Al-2% and Al-5% Cu alloys.

Task Description:

The theoretical work will consist of the following tasks:

1. Develop a formulation to describe the rheology of the particular two-phase equiaxed/columnar systems of interest (dendritic and eutectic);
2. Develop an analytical solution for microsegregation for the case of an open system;
3. Develop a formulation for thermosolutal and shrinkage flow that includes description of both macro- and micro-segregation;
4. Couple the macro-transport to micro-transport through description of solidification kinetics;
5. Develop a numerical code to solve the above algorithm;
6. Evaluate the validity of the closed system microsegregation model for the case of low-g environment.

The open system model will be used in validation in conjunction with both high-g and low-g experiments. In addition, by turning off the shrinkage flow and/or the solid-liquid relative motion flows, the relative effects of these flows can be evaluated. The closed system model should come reasonably close to the low-g experiments. Validation of the models will be done through experimental measurement of solute concentration at the macro- and micro-scale level, and of the temperature distribution.

The equipment that will be used for the experiments is NASA's Isothermal Casting Furnace that has a temperature range of 100 to 1350 °C, and quenching rate capabilities of 1 to 50 °C/s. This furnace will be flown on the DC-9 aircraft. The samples will be melted before the low-g period of the flight, and solidified during the 25 seconds of low-g. Parallel experiments will be conducted on the ground.

Task Significance:

At the microscale level, the assumption that mass transport is purely diffusive is quite reasonable, and thus, a closed system may be a good approximation for certain alloy systems solidifying under terrestrial gravity. This assumption is even more valid when considering low-gravity (low-g) solidification. However, for most alloy systems the influence of fluid flow caused by thermal and solutal convection cannot be ignored. During

solidification of a multicomponent alloy, buoyancy-driven fluid flow occurs due to the temperature and concentration gradients. Even in upward directional solidification it is difficult to avoid horizontal temperature gradients since the container walls are not perfectly adiabatic. Accordingly, there is a need to further develop the model to address the open system case.

Progress During FY 1996:

During FY96 two compositions of Al-Cu alloys have been investigated, Al-2% Cu and Al-5% Cu, using two different cooling rates. Vertical sections of the cast ingots were polished and etched to examine the micro- and macrostructure. Evaluation of the composition of each sample was done using the Electron Microprobe (JXA-8600) at the University of Alabama in Tuscaloosa. These measurements were done with a 200 μm diameter beam and 200 μm between each measurement, in the central vertical section of each sample. Significant variations in the micro-/macrostructure, and in the composition between low-g and ground solidified samples, as well as between samples solidified at various cooling rates were found. Low-g samples have larger primary dendritic arm spacing than ground samples. Also, they have more homogeneous distribution. As expected, a higher cooling rate resulted in a finer primary dendrite arm spacing than low cooling rate. The secondary dendrite arm spacing is about the same for all samples, regardless of the gravity level or cooling rate (between 10 to 25 μm). The variation of composition in the ground samples shows a more uniform behavior and lower level of macrosegregation than in low-g. In low-g, the variation of composition has a pattern similar to the one obtained by other researchers which have done ground experiments with upward solidification direction. The comparison between different cooling rates permits to conclude that the behavior is opposite to the one expected, meaning that, in low-g, higher cooling rate produces higher macrosegregation. Consequently, seven more samples were produced in low-g conditions using two different new cooling rates to investigate this unexpected behavior. This ongoing research would give a better understanding of the effect of gravity on the macrosegregation problem. The recently developed Chang-Stefanescu model for macrosegregation, was applied to explain the differences in macrosegregation. As expected, significant differences were found.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	1	MS Degrees:	0
PhD Students:	1	PhD Degrees:	1

TASK INITIATION: 8/94 EXPIRATION: 8/96

PROJECT IDENTIFICATION: 962-25-08-34

NASA CONTRACT NO.: NCC8-59

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Chang, S., and Stefanescu, D.M. A model for inverse segregation: The case of directionally solidified Al-Cu alloys. *Acta mater.*, vol. 44, no. 6, 2227-2235 (1996).

Chang, S., and Stefanescu, D.M. A model for macrosegregation and its application to Al-Cu castings. *Metallurgical and Materials Transactions*, vol. 27A, 2708-2721 (1996).

Proceedings

Stefanescu, D.M., Leon-Torees, J., Sen, S., and Dhindaw, B.K. "Influence of gravitational acceleration on the macrosegregation of Al-Cu alloys." 3rd International Conference on Modeling of Casting and Solidification Processes, Beijing, China, December 1996.

Test of Magnetic Damping of Convective Flows in Microgravity

PRINCIPAL INVESTIGATOR: Dr. Frank R. Szofran

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Cobb, S.D.

NASA Marshall Space Flight Center (MSFC)

Robinson, M.B.

NASA Marshall Space Flight Center (MSFC)

Volz, M.P.

NASA Marshall Space Flight Center (MSFC)

Motakef, S.

CAPE Simulations, Inc.

Task Objective:

The objectives of this study are: to test experimentally the validity of the modeling predictions applicable to the magnetic damping of convective flows in conductive melts as this applies to the directional solidification of semiconductor and metallic materials in the reduced gravity levels available in low Earth orbit; and to assess the effectiveness of magnetic fields in reducing the fluid flows occurring in these materials during space processing that result from density gradients (driven by the residual steady-state acceleration or g-jitter) or surface tension gradients (Marangoni flow). To achieve these fundamental objectives, the following specific objectives will be pursued:

- To determine the relative effectiveness of an axial magnetic field in suppressing convective flows in 1g driven by gravity, vibration, or surface tension gradients;
- To test the validity of magnetohydrodynamic modeling predictions in characterizing the effectiveness of an axial magnetic field for suppressing convective flows in 1-g.

Task Description:

To achieve the objectives of this investigation, we carried out a ground-based program using a carefully chosen set of materials. Some of these materials have been intensely studied in environments that have not simultaneously included both low gravity and an applied magnetic field. These include a dilute alloy (Ga-doped Ge) in which solutal effects will be negligible and the solid solutions Ge-Si and InSb-GaSb with liquid density ratios of 2.18 and 1.07, respectively. Thus, during Bridgman-Stockbarger solidification with the solid on the bottom, Ge-Si has a strongly stabilizing solutal density variation and InGaSb is very mildly stabilizing with previous results showing substantial. All three systems were processed by the Bridgman method using 8mm diameter samples.

Task Significance:

During directional solidification of semiconductors, generation of destabilizing temperature gradients in the melt is unavoidable, resulting in buoyancy-induced convective mixing of the liquid phase. On Earth this convective mixing is generally very intensive and interferes with segregation of melt constituents at the growth front leading to less than optimum quality crystals. Crystal growth in space provides the opportunity to reduce the convective intensity and, for some classes of systems and charge sizes, achieve mass transfer diffusion-controlled growth. Magnetic damping of convection in electrically-conductive melts, however, can be used to provide a higher degree of control on convection in the melt. Thus our understanding of convective influences can be further advanced, and our ability to interpret space experimental results may be significantly improved.

Progress During FY 1996:

Nominally, this project was completed at the end of FY95; however, some funds remained and were used to carry on this work until funds from a new proposal to continue the work became available midway through FY96. Experimental work included Bridgman growth and crystal characterization. The numerical modeling effort also continued. Collaboration with the Crystallographic Institute of the University of Freiberg, Germany continued and plans were made to conduct another series of experiments with the Freiburg mirror furnace in the 5 Tesla magnet at MSFC.

Significant accomplishments during the first half of FY96 include:

- Recognition of the importance of the thermal field in conjunction with an applied magnetic field in order to most reliably achieve diffusion controlled growth conditions. Preliminary design concepts for a new furnace to improve the thermal field were developed.

- Implementation of current pulse interface demarcation as an alternative to mechanical interface demarcation. Current pulses in a magnetic field generally cause a mechanical disturbance and the relative merits of mechanical only versus current demarcation are still being considered.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/92 EXPIRATION: 3/96

PROJECT IDENTIFICATION: 962-35-24

RESPONSIBLE CENTER: MSFC

Magnetic Damping of Solid Solution Semiconductor Alloys

PRINCIPAL INVESTIGATOR: Dr. Frank R. Szofran

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Benz, K.W.

Kristallographisches Institut

Cobb, S.D.

NASA Marshall Space Flight Center (MSFC)

Cröll, A.

Kristallographisches Institut

Dold, P.

Kristallographisches Institut

Lehoczky, S.L.

NASA Marshall Space Flight Center (MSFC)

Motakef, S.

CAPE Simulations, Inc.

Task Objective:

The objectives of this study are: (1) to experimentally test the validity of the modeling predictions applicable to the magnetic damping of convective flows in conductive melts as this applies to the directional solidification and floating zone growth of solid solution semiconducting materials; and, (2) to assess the effectiveness of steady magnetic fields in reducing the fluid flows occurring in these materials during space processing that result from density gradients (driven by the residual steady-state acceleration or g-jitter) or surface tension gradients (Marangoni flow).

Task Description:

To achieve the objectives of this investigation, we will continue to carry out a comprehensive program in the Bridgman and floating-zone configurations using the solid solution alloy system Ge-Si. This alloy system is the subject of much work at the participating organizations and has been studied extensively in environments that have not simultaneously included both low gravity and an applied magnetic field. The study will include dilute alloys (doped Ge and doped Si) in which solutal effects will be negligible as well as the solid solutions. During Bridgman-Stockbarger solidification with the solid on the bottom, Ge-Si (or GeSi or $\text{Ge}_{1-x}\text{Si}_x$) has displayed axial compositional variations which appear to be diffusion-controlled although the radial compositional variations indicate significant convection. The Ge-Si system will be float-zoned both to study the effects of magnetic suppression of Marangoni convection with uncoated samples and to study thermosolutal convection with oxide-coated samples (Si only). The coated samples will be doped in such a way as to provide a method to assess the effects of a magnetic field on laminar convection. The comparison of the Bridgman-grown and float-zoned results will aid significantly in the determination of the sensitivity of the growth processes to magnetic damping and residual convection.

Task Significance:

During Bridgman or floating zone growth of semiconductors, generation of destabilizing temperature gradients in the melt is unavoidable, resulting in buoyancy-induced convective mixing of the liquid phase. On Earth this convective mixing is generally very intensive and interferes with segregation of melt constituents at the growth front. Crystal growth in low Earth orbit provides the opportunity to reduce the buoyancy-induced convective intensity and, for some classes of systems and charge sizes, mass transfer diffusion-controlled growth may be achieved if the residual acceleration direction and magnitude can be controlled. However, calculations and recent flight experiment results clearly indicate that simply reducing the steady-state acceleration to values achievable in low-Earth orbit will not provide diffusion controlled growth conditions for solid solution melts $\approx 1\text{cm}$ in diameter if accelerations transverse to the growth axis are not controlled. This study will provide the Earth-based database necessary to assess the effectiveness of magnetic field suppression of disturbances caused by residual accelerations aligned or not aligned with the normal to the solid-liquid interface and by random, non-steady accelerations (g-jitter). Also, it will show whether the current state of the art in numerical modeling can be used to predict the behavior of electrically conductive melts over a range of applied magnetic fields.

Progress During FY 1996:

A series of gallium-doped germanium samples were grown at different magnetic fields, using hot-pressed boron nitride, pyrolytic boron nitride, and graphite ampoules. Current pulse interface demarcation was used in all samples in this series to determine the growth interface shape and microscopic growth rate. The mechanical disturbance necessarily introduced by a current pulse in a magnetic field, although carefully minimized, was still detectable in the samples as a ringing or sloshing which caused striations in addition to those caused by the current pulse. The relative merits of purely mechanical demarcation versus current pulse demarcation in a magnetic field are still being investigated.

In collaboration with the Co-Investigators from the Crystallographic Institute (KI) in Freiburg, a second series of float-zone samples and a series of Bridgman samples were grown in the KI mirror furnace installed in one of the 5 Tesla magnets at MSFC. Most of the float zone samples were silicon with various dopants, however, one germanium and one silicon germanium alloy were grown successfully. The Bridgman samples included both germanium and silicon-germanium alloys. These samples are currently being analyzed including the germanium Bridgman sample grown in zero field as a control and which grew for some 2 cm without contact with the ampoule. The possibility of this happening in unit gravity had been predicted by Professors Regel and Wilcox at Clarkson University although they expected it to happen when a sample was grown in a high magnetic field.

STUDENTS FUNDED UNDER RESEARCH:**TASK INITIATION:** 3/96 **EXPIRATION:** 4/00**PROJECT IDENTIFICATION:** 962-21-22**NASA CONTRACT NO.:** NAG8-128**RESPONSIBLE CENTER:** MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Proceedings**

Dold, P., Cröll, A., Szofran, F., Kaiser, Th., and Benz, K.W. "Growth of semiconductor crystals: comparison between the effect of microgravity and magnetic fields." Proceedings of the Third China-Japan Workshop on Microgravity Science, Xian, China, October, 1996.

Presentations

Dold, P., Cröll, A., Szofran, F., Kaiser, Th., and Benz, K.W. "Growth of semiconductor crystals: comparison between the effect of microgravity and magnetic fields." Presented at the Third China-Japan Workshop on Microgravity Science, Xian, China, October, 1996.

Szofran, F.R. "Magnetic damping of solid solution semiconductor alloys." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Szofran, F.R., Motakef, S., and Volz, M.P. "Bridgman growth of Ge:Ga in a static magnetic field." Presented at the Tenth American Conference on Crystal Growth, Vail Colorado, August, 1996.

The Features of Self-Assembling Organic Bilayers Important to the Formation of Anisotropic Inorganic Materials in Microgravity Conditions

PRINCIPAL INVESTIGATOR: Dr. Daniel R. Talham

University of Florida

CO-INVESTIGATORS:

Adair, J.H.

University of Florida

Task Objective:

The objective of this program is to develop a fundamental understanding of the growth of anisotropic particles at organic templates, with emphasis on the chemical and structural aspects of layered organic assemblies that contribute to the formation of anisotropic inorganic particles. Target systems include both metal particles important to conductive pathways in microelectronics such as Ag/Pd alloys and Pt, and II-IV semiconductors such as CdSe and CdS. This project aims to extend the current level of understanding of particle formation at micellar structures to the preparation of anisotropic inorganic particles.

Task Description:

We will make extensive use of model membrane systems prepared by Langmuir-Blodgett methods in order to efficiently survey possible template systems and establish the important chemical and geometric features of the templates that influence particle growth. It is planned to use what is learned on the model systems to develop larger-scale preparations of the targeted inorganic materials at bilayer structures formed from "oil-in-water" segregated phase systems. It is these systems that will eventually lead to high yield, monodisperse preparations. Inorganic ions trapped within the aqueous region of the templating structures will be reacted to form either metal particles or metal salt particles. Results from the surface confined studies will be continuously utilized in the design and choice of solution micellar systems as they are tailored to the desired inorganic materials. When going from the model systems toward larger scale solution preparations, the fundamental chemical and geometrical templating interactions will be in competition with effects caused by convection and in some cases sedimentation, and the limits of these procedures will be masked by gravity effects. Systems suitable for investigation under microgravity conditions will be developed.

Task Significance:

There is a growing need for inorganic anisotropic particles in a variety of materials science applications. Structural, optical, and electrical properties can be greatly augmented by the fabrication of composite materials with anisotropic microstructures or with anisotropic particles uniformly dispersed in an isotropic matrix. Examples include structural composites, magnetic and optical recording media, photographic film, certain metal and ceramic alloys, and display technologies including flat panel displays.

Progress During FY 1996:

Nanometer-sized composite particles (nano-composites) with core-shell structures have been prepared by arrested precipitation of metal or semiconductor clusters in reverse micelles, followed by hydrolysis and condensation of organometallic precursors in the microemulsion matrices. Temporally discrete nucleation and growth at elevated temperature (70 °C) give the resulting particles a narrow size distribution and defined crystallinity. Both the size of the core particles and the thickness of the coating layers can be varied by controlling processing parameters such as the ratio of water to surfactant and the ratio of water to organometallic precursors. By controlling the pH conditions and aging temperatures a transparent gel composed of nanometer-sized inorganic clusters has been obtained.

Quantum confinement effects on the cadmium sulfide nanosize clusters and nano-composites have been observed. For the silver metal clusters and nano-composites the shift of the absorption peak at the surface-plasmon resonance frequency due to classical limited mean-free path of the conduction electrons or quantum size effects has been observed. The enhanced third-order nonlinear susceptibility of the silver nano-composites results from the local field enhancement and size-effects, which has been experimentally demonstrated by an optical phase conjugation technique.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 4/96 **EXPIRATION:** 4/00**PROJECT IDENTIFICATION:** 962-21-49**NASA CONTRACT No.:** NAG8-124**RESPONSIBLE CENTER:** MSFC

Microporous Membrane and Foam Production by Solution Phase Separation: Effects of Microgravity and Normal Gravity Environments on Evolution of Phase Separated Structures

PRINCIPAL INVESTIGATOR: Dr. John M. Torkelson

Northwestern University

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this research is to develop a quantitative understanding of the microstructure formation in glassy, polymeric microporous membranes and foams produced via thermally induced phase separation. In particular, this study will work toward delineating the role of gravity (resulting in buoyancy-driven flows yielding macroscopic layering of phases) or the absence thereof in both the early-stage phase separation mechanisms, spinodal decomposition versus nucleation and growth, and the later effects of coarsening, by Ostwald ripening and/or hydrodynamic flow. Coarsening effects will be studied quantitatively by experimental determination of the growth in pore size over time as a function of quench depth, polymer molecular weight and concentration, surface tension, etc., in near-critical and off-critical composition phase separation processes. Comparisons to expectations based on Ostwald ripening and hydrodynamic flow mechanisms of coarsening will be made. By developing a quantitative understanding of the thermodynamics and kinetics of polymer solution phase separation processes, both in terms of gravitational effects and the more ordinary effects of polymer/molecular weight/solvent/concentration/quench temperature/quench time conditions, it may be possible to optimize microporous membrane and foam structure and performance. Comparisons between coarsening effects in 3-dimensional and 2-dimensional environments, the latter expected to behave as if they are in a microgravity environment even if the polymer and solvent have differing densities and the experiments are done on earth, will also be undertaken. In particular, comparisons of experimental results of 2-dimensional coarsening behavior with predictions from theory and numerical simulation will be made.

Task Description:

A microgravity environment will be simulated by use of isopycnic (iso-density) solutions of polystyrene in diethyl malonate, diethyl oxalate and related solvents, which upon thermally induced phase separation do not exhibit any macroscopic layering effects on the time frame of a day to a week. Comparisons will be made to conventional, nonisopycnic polystyrene solutions. Early-stage spinodal decomposition effects will also be investigated by comparing the experimental temperature dependence of pore size to predictions from the linearized Cahn-Hilliard theory for spinodal decomposition. Measurements of the average pore size and pore-size distribution in membranes and foams produced by thermally induced phase separation will be characterized by scanning electron microscopy and mercury intrusion porosimetry. Comparisons of the growth rate in pore size observed from the three-dimensional membranes will be made to *in situ* measurements of phase separation and coarsening in polymer solutions by optical microscopy; the thin nature (1 to 10 microns between the base slide and cover plate) of the solutions yields two-dimensional coarsening effects when the phase separated droplets are equivalent to or larger than the film thickness. In particular in the case of two-dimensional coarsening, effects of composition (off-critical, near-critical, and critical compositions), film thickness, polymer molecular weight, solvent viscosity and quench depth will be explored.

Task Significance:

The effects of gravity in the production of microporous membranes and foams from phase separated polymer solutions will be studied quantitatively for the first time. By accessing microgravity conditions, it will be possible to study critically how the phase domain growth rate during coarsening compares to theories, including those related to the Ostwald ripening mechanism and the hydrodynamic flow mechanism of coarsening. From a scientific standpoint, by simulating microgravity conditions it will be possible to test for the first time the evolution of coarsened microstructure in polymer solutions over many orders of magnitude in phase separation time and to determine how gravity-driven flows affect this evolution. From a technological standpoint, the microgravity environment using the isopycnic solution will allow determination of how space processing of microporous polymer membranes and foams may result in materials unobtainable or obtainable only for limited polymer species (where isopycnic solutions can be found) in a conventional terrestrial environment. These studies will also allow for a determination of how novel materials may be developed in 2-dimensional phase separation. As buoyancy

driven flows should occur only in 3-dimensional phase separation, 2-dimensional phase separation may be expected to simulate microgravity environments even on earth regardless of the solvent and polymer densities. These studies will also be important from a basic scientific standpoint in that much theoretical and numerical simulation work has been done on the issue of two-dimensional coarsening, but almost no experimental studies have been undertaken to date.

Progress During FY 1996:

Polymer solutions of various compositions have been phase separated in two dimensions in order to monitor the growth rate of the domain size, d , associated with coarsening in restricted dimensions. These two-dimensional coarsening studies, which are not subject to gravity-driven macroscopic phase separation, have also been compared to three-dimensional coarsening of phase-separating polymer solutions, where gravity-driven buoyancy effects can become important on short time scales if the difference in polymer and solvent densities are significant enough.

We completed the first experimental two-dimensional coarsening study of any type to demonstrate that the domain-size growth rates are dependent on overall composition (specifically, distance from the "critical" point) and that there is substantial agreement with theoretical expectations. In particular, for near-critical systems, a crossover in growth rates occurs, with d growing as $Kt^{1/3}$ at short times and d growing as $t^{2/3}$ at long times, where t is coarsening time. In contrast, for off-critical solutions, d grows approximately as $Kt^{1/3}$ without a crossover to a faster coarsening rate. Both results agree well with theory and numerical simulation and are the first experimental confirmations of the theory. In the case of off-critical solutions, coarsening occurs predominantly by Ostwald ripening rather than coalescence; in contrast, the near-critical coarsening shows, at early stages, both Ostwald ripening and coalescence, with the later-stage, after-crossover coarsening being consistent with a flow-driven coarsening mechanism. In the case of near-critical systems, the crossover domain size decreases with increasing quench depth in a manner consistent with a transition from a thermally-driven to a flow-driven coarsening mechanism. In general, the factor K increases with area fraction of the dispersed phase for a given off-critical or near-critical system, in qualitative agreement with theory. Both average and crossover domain sizes increase with increasing film thickness, and coalescence is significantly dependent on film thickness while Ostwald ripening is not. Substrate polarity effects were investigated showing that substrate polarity does not greatly affect off-critical coarsening, although near-critical coarsening (particularly near the crossover in growth rate) is greatly affected. Solvent viscosity was varied by more than an order of magnitude, with no significant effect on coarsening in off-critical or near-critical systems. Effects of polymer molecular weight are tied into the molecular-weight dependence of interfacial tension, a point of current investigation.

These two-dimensional coarsening growth-rate effects compare favorably to the results obtained by us in three-dimensional coarsening studies using similar polymer-solvent systems, where, with small quench depths, $d \approx t^{1/3}$ at short times with a crossover at longer times to a linear (1st) power in time. In both two-dimensional and three-dimensional cases, the short time effects ($1/3$ power) are consistent with coarsening by Ostwald ripening and/or coalescence while the long time effects ($2/3$ power in two-dimensional and 1st power in three-dimensional) are consistent with the hydrodynamic flow mechanism of coarsening. In the case of larger quench depths, the growth-rate exponent at short times was found to be less than $1/3$ and decreasing with increasing quench depth. We believe that this may be due to the deeply-quenched phase-separating polymer solutions not yet having reached the equilibrium phase compositions during the early stages of coarsening. The theory predicting the $1/3$ growth-rate exponent explicitly assumes that phase compositions have reached their equilibrium values; other apparent growth-rate exponents may result if this condition does not hold. In support of this conclusion, when two-dimensional systems are phase separated under conditions where the phase compositions (and therefore the fractional phase volumes) are changing, growth-rate exponents other than predicted by theory (assuming constant phase compositions) are obtained. Determination of whether the fractional phase volumes are changing during the early stages of three-dimensional coarsening are currently being studied via analysis of microporous membrane and foam structures obtained from thermally induced phase separation of polymer solutions. Work is also in progress regarding the long-term evolution of phase-separated and coarsened microstructure of membranes under conditions where isopycnic solutions where effects of gravity are minimized.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 6/94 EXPIRATION: 6/96

PROJECT IDENTIFICATION: 962-21-08-23

NASA CONTRACT No.: NAG8-106

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Haas, C.K., and Torkelson, J.M. 2D vs. 3D coarsening in phase-separated polymer solutions: Dependence on distance from criticality and interfacial tension. ACS Polymer Preprints, vol. 36, no. 2, 360 (1995).

Haas, C.K., and Torkelson, J.M. 2D coarsening in phase-separated polymer solutions: Dependence on distance from criticality. Phys. Rev. Lett., vol. 75, 3134 (1995).

Dynamically-Induced Nucleation of Deeply Supercooled Melts and Measurement of Surface Tension and Viscosity

PRINCIPAL INVESTIGATOR: Dr. Eugene H. Trinh

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Ohsaka , K.

Jet Propulsion Laboratory (JPL)

Task Objective:

The major topics of interest of this research project are the study of dynamic pressure as a means to induce solid phase nucleation in the undercooled liquid state and the development of novel methods of measuring the surface tension and viscosity of deeply undercooled liquids with moderate and high viscosity. The experimental approach is based on previously developed single droplet positioning/levitation methods combined with the ultrasonic technique of trapping and driving gas bubbles into large amplitude volume oscillations. The same single particle levitation approach will be implemented in the development and validation of a rotation-based method to measure the surface tension and viscosity. The ultimate goals of this study are to experimentally verify the hypothesis that large dynamic pressure excursions can trigger the liquid-solid phase transition, and to gather surface tension and viscosity data for deeply undercooled melts to test current theories for the liquid state. The required high intensity fields for sample levitation and trapping in 1-g and the modification of sample positions due to gravity introduce substantial error in the measurements of the relevant parameters. The performance of microgravity investigations will not only lead to more precise measurements, but it will also allow theoretical modeling of the actual experimental conditions.

Task Description:

In order to test the hypothesis of pressure-induced nucleation, we plan to drive a single bubble immersed in an undercooled liquid into large amplitude oscillations in order to generate well localized, but violent pressure fluctuations. A systematic study aiming to correlate these monitored bubble oscillations to the onset of nucleation in a well defined spatial region will be carried out. The bubbles will be artificially introduced via either hydrolysis or focused laser irradiation, and they will be driven into oscillation by an ultrasonic standing wave established in a small volume of undercooled liquid. This liquid host will be in the form of a single droplet, or it will be contained in a specially treated cavity. The steady-state motion of the bubble will be monitored through strobed illumination as well as laser light scattering, thus providing a real-time diagnostic of the time-dependent pressure variations in the vicinity of the oscillating bubble. The statistics relating to the onset of solidification of the liquid will thus be compiled to extract a potential correlation between the pressure fluctuations and the nucleation events.

Currently used non-invasive methods of surface tension measurement for the case of undercooled liquids generally rely of the quantitative determination of the resonance frequencies of drop shape oscillations, of the dynamics of surface capillary waves, or of the velocity of streaming flows. These methods become quickly ineffective when the liquid viscosity rises to a significant value. An alternate and accurate method which would be applicable to liquids of significant viscosity is therefore needed. We plan to develop such a capability by measuring the equilibrium shape of levitated undercooled melt droplets as they undergo solid-body rotation. The experimental measurement of the characteristic point of transition (bifurcation point) between axisymmetric and two-lobed shapes will be used to calculate the surface tension of the liquid. Such an approach has already been validated through the experimental verification of numerical modeling results. The experimental approach will involve levitation, melting, and solidification of undercooled droplets using a hybrid ultrasonic-electrostatic technique in both a gaseous as well as a vacuum environment.

A shape relaxation method will be investigated in order to derive a reliable method to measure the viscosity of undercooled melts. The analysis of the monotonic relaxation to equilibrium shape of a drastically deformed and super-critically damped free drop has been used to derive interfacial tension of immiscible liquid combinations where one of the component has high viscosity. A standard approach uses the initial elongation of a droplet through shear flows, but an equivalent method could involve the initial deformation of a drop levitated in a gas by ultrasonic radiation pressure, electric stresses, or even solid body rotation. The dynamic behavior of the free drop relaxing

back to equilibrium shape has already been modeled, and its characteristic time dependence will provide a quantitative means to evaluate the liquid viscosity.

Task Significance:

Many processes and products derived from materials manufacturing involve the supercooling of liquids, and some specific enhanced properties of the materials arise only because the liquid has been solidified while in a deeply supercooled state. The ability to supercool a melt is therefore a required capability in these cases, and the knowledge of the controlling parameters allowing the access to this deep supercooled state is therefore extremely valuable. Similarly, because access to this non-equilibrium state is difficult, the measurement of its thermo-mechanical properties is also complicated. The development of novel measurement techniques which maximize access to the supercooled range is therefore also required.

Progress During FY 1996:

This task has just been initiated, and two approaches are currently being developed:

- The first experimental task involves the trapping of resonantly driven oscillating bubbles in a supercooled liquid. We are currently designing an apparatus which would allow the supercooling of a small volume of transparent liquid (2-3 ml) and the trapping of a small air bubble (20 to 50 microns diameter). A dual frequency approach using a standing and a traveling wave will allow the trapping of the bubble and its drive into large amplitude radial oscillations. The visualization and monitoring of the bubble oscillations and the associated pressure field within the supercooled liquid will be carried out through light scattering and high magnification video observation.
- The second approach involves the development of an apparatus for the supercooling of levitated droplets and their rotation under a controlled rate. An acoustic-electrostatic hybrid technique will be the most likely approach with a combination of laser spot heating and isothermal controlled chamber sample thermal control.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/96 EXPIRATION: 9/99

PROJECT IDENTIFICATION:

RESPONSIBLE CENTER: MSFC

A Proposal to Further Investigate the Influence of Microgravity on Transport Mechanisms in a Virtual Space Flight Chamber

PRINCIPAL INVESTIGATOR: Dr. James D. Trolinger

MetroLaser, Inc.

CO-INVESTIGATORS:

Lal, R.

Rangel, R.

Witherow, W.

Alabama A&M University

University of California at Irvine

NASA Marshall Space Flight Center (MSFC)

Task Objective:

The first objective is to advance the understanding of microgravity effects on crystal growth, convection in materials processing in the Space Shuttle environment, and complex transport phenomena at low Reynolds numbers. This objective will be achieved through the use of existing holographic data recorded during the IML-1 space flight. Much of the convection present in these recordings is connected with thermal and concentration gradients related to crystal growth and is driven by g-jitter, residual g and other sources not yet understood.

The second objective is to design a space flight experiment that exploits the "virtual space chamber concept." The experiment will be a crystal-growth-in-space experiment that can be conducted in a simplified chamber and operated in a GAS can or flight deck locker. Anticipated crystal candidates are: 1) various protein crystals; 2) LAP; 3) KDP; and, 4) LiIO_3 .

Task Description:

Extract additional data from the IML-1 holograms to support the development of physical models of particle/fluid interactions important to crystal growth in space.

1. Assess remaining useful data in the IML-1 holograms.
2. Extract additional supporting data for measurements, conclusions, and unanswered questions that have already resulted from the IML-1 holograms.
3. Examine additional data types from IML-1 holograms not already considered, such as three dimensional convection, and particle interaction, particle/wall interaction.
4. Analyze and interpret newly generated IML-1 data with newly developed particle/fluid model.

Perform analysis and ground-based experiments that can lead to the development of a space experiment that incorporates the holographic virtual space chamber concept.

5. Produce a preliminary experiment design which consists of:
 - a. Acceleration measurements.
 - b. Microgravity measurements (residual gravity / g-jitter).
 - d. Crystal growth monitoring.
 - e. Particle movement with force field.
 - f. Preliminary selection of crystal, fluid, and particle type/size.
6. Produce a preliminary instrument design based on the holographic virtual space chamber concept.
7. Model the proposed instrument.
8. Breadboard and test the instrument.
9. Perform ground crystal growth demonstration.
10. Design a flight package.
11. Produce final report and recommendations.

Task Significance:

Previous work has convinced us that a considerable amount of valuable information that is relevant to materials processing in space is available in the existing NASA spaceflight data. Accessing the data in holograms made in space will prove to be an extremely cost effective way to promote the understanding of convection and microgravity

effects on materials processing in space. Our technical approach, therefore, is designed to exploit existing NASA space flight data to provide knowledge about microgravity influences in materials processing. This knowledge will be used to design a new space flight experiment that would be superior to any existing flight hardware in its capabilities to both monitor critical crystal growth parameters and directly measure microgravity effects such as residual gravity and g-jitter. By studying these effects, fluids and materials researchers will gain a greater understanding of the conditions, environment, and physics in the available microgravity environments. This will greatly enhance the capability of any spaceborne platform intended for materials processing.

Progress During FY 1996:

The project began in 1996. During the first quarter the PI met with the project officer, Dr. Roger Kroes, attended the Microgravity Materials Science conference in Huntsville and presented a poster paper. The project team met twice to firm up plans, coordinate the tasks, go over the schedule, and integrate the ideas of all participants. Plans were finalized for theoretical modeling and experimental data generation from existing holograms. We decided to explore specific independent cases of particles in the microgravity environment including the following: particles not influenced by other particles or by walls, particles influenced by other particles, and particles influenced by walls and crystal growth. To augment the study we chose to first assemble a complete data base of all particle locations and sizes for the IML-1 chamber. This would allow us to easily sort special cases for additional high resolution tracking and analysis. To simplify new data extraction a request to transfer (from MSFC) the data extraction task during the first year to the MetroLaser Irvine laboratory was made and granted. A reconstruction system was assembled for this purpose using both in-house MetroLaser equipment and equipment available at MSFC. Image processing algorithms were examined and refined for use in data extraction and for automating the process.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 6/00

PROJECT IDENTIFICATION: 962-21-23

NASA CONTRACT No.: NAS8-408

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Trolinger, J.D., Lal, R.B., McIntosh, D., and Witherow, W.K. Holographic Particle Image Velocimetry in the First International Microgravity Laboratory aboard the Space Shuttle Discovery. Applied Optics, vol. 35, no. 4, 681-689 (1996).

Proceedings

Trolinger, J.D., Rangel, R., and Lal, R. "Particle Mechanics and G-jitter Observations in the IML-1 Spaceflight." AIAA 96-0504, 34th Aerospace Sciences Meeting, January 1996.

Fundamentals of Mold-Free Casting Experimental and Computational Studies

PRINCIPAL INVESTIGATOR: Prof. Grétar Tryggvason

University of Michigan

CO-INVESTIGATORS:

Ceccio, S.L.

University of Michigan

Jacqmin, D.

NASA Lewis Research Center (LeRC)

Task Objective:

The task objective is to:

1. Provide the scientific knowledge necessary to operate a net-shape drop and spray casting facility by a computer designed and optimized process. In addition to its importance for earth based manufacturing, such knowledge will allow the operation of a space based facilities by computer programs developed on Earth.
2. Develop a detailed understanding of the fluid mechanics, heat transfer, and solidification of drops splatting on a solid surface or a layer of other drops, that can be used to predict the microstructure of solids formed by such depositions.

Task Description:

The project has both an experimental and a computational part. The experiment will consist of a facility that will allow drops of controlled size and velocity to be deposited on a flat substrata where they solidify. The numerical part will build on techniques developed under previous NASA support for accurate simulations of drop motion. By a careful comparison of the numerical and the experimental results, we expect to be able to identify the key physical aspects of the process that must be included in the numerical model so that it yields accurate results, yet is sufficiently fast to be of practical use. To scale-up of the drops to allow more detailed observations of the process, we expect eventually to conduct the experiments in a low gravity environment where the drops can be made larger and the velocities smaller, while keeping the essential balance of physical effects the same as for the small drops that will be used in the actual production of artifacts.

Task Significance:

Moldfree casting by precision controlled deposition of drops of molten metal is an emerging manufacturing process with considerable promise for rapid prototyping and the production of high quality, custom artifacts. A detailed understanding of the process, and the ability to predict the effect of the controlling parameters, is essential if the technique is to reach its full potential.

Progress During FY 1996:

- 1) We have developed the capability to simulate the deformation of liquid metal drops as they are deposited on a substrate. These are fully resolved, three dimensional calculations.
- 2) These simulations have been extended to solidification of drops of pure material, and we expect that these simulations can be extended to include the solidification of binary solutions.
- 3) We have developed a drop producing apparatus which is capable of producing individual drops of liquid metal. We are modifying the device to insure its function in the microgravity environment.
- 4) We have successfully compared the numerical and experimental results for solidifying and non-solidifying liquid metal drops.
- 5) The traverse and cooling system for the substrate has been completed, and a vacuum chamber design has been completed.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0

MS Students: 0

PhD Students: 1

TASK INITIATION: 7/94 EXPIRATION: 7/96

PROJECT IDENTIFICATION: 962-25-05-28

NASA CONTRACT NO.: NCC3-355

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

NASA Tech Briefs

Tryggvason, G., Ceccio, S. L. and Jacqmin, D., Fundamentals of mold free casting: experimental and computational studies. NASA Tech Brief, 4735, p. 724 (1996).

Presentations

Ceccio, S. L., Tryggvason, G., Han, J., Che, J. and Juric, D., "Fundamentals of mold free casting: experimental and numerical studies." poster presentation at the Microgravity Materials Science Conference, Huntsville, Alabama, 1996.

Tryggvason, G., Juric, D., Han, J. and Ceccio, S.L., "Direct numerical simulations in material processing." in Space Processing of Materials, Narayanan Ramachandran, Editor, Proc. SPIE 2809, pp. 178-184 (1996).

Electromagnetic Field Effects in Semiconductor Crystal Growth

PRINCIPAL INVESTIGATOR: Dr. Martin P. Volz

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Mazuruk, K.

Universities Space Research Associates (USRA)

Waring, D.A.

NASA Marshall Space Flight Center (MSFC)

Dulikravich, G.S.

Pennsylvania State University

Task Objective:

The objectives of this investigation are the following:

1. To investigate the effects that combined electric and magnetic fields have on gravitationally-driven fluid flow processes during the bulk growth of selected semiconductor alloys.
2. To examine the criteria for the onset of thermal instability as a function of electric, magnetic, and gravitational field strength in electrically conducting liquids via theoretical analysis, computer calculations, and laboratory experiments.
3. To assess the possibility of using externally applied magnetic and electric fields to influence fluid motion in the melt, the rate of solid phase accrual, and the shape of the solid/liquid interface during solidification experiments both on earth and in a low gravity environment.

Task Description:

A series of specific tasks are planned to achieve the proposed objectives. A model growth cell will be developed and placed inside of a rotating magnetic field. *In situ* temperature measurements will be made using gallium as a model material. Both zone-melting and vertical Bridgman thermal profiles will be applied and the onset of thermal fluctuations will be measured as a function of rotating magnetic field strength. Computer modeling of the above system will be accomplished by using a three-dimensional mathematical model which takes into account both magnetohydrodynamic and electrohydrodynamic phenomena. The model predictions will be compared with the experimental results from the model growth cell.

Task Significance:

Electromagnetic fields can interact with electrically conducting melts and substantially affect their fluid flow processes. Indeed, the intriguing possibility exists of using combined electric and magnetic fields to control fluid flow in the melt during the directional solidification of semiconductor alloys. The significance of this study is to gain a basic understanding of the possible interactions that combined electric and magnetic fields can have on fluid flow processes during semiconductor crystal growth.

Progress During FY 1996:

We have developed and refined a new analytical formulation of combined electro-magnetohydrodynamics (EMHD) and have shown the inconsistencies and shortcomings of the existing separate electro-hydrodynamic and magneto-hydrodynamic theories. The new model consists of a system of twelve coupled non-linear partial differential equations in the case of a three-dimensional flow. The model is valid for multi-dimensional unsteady viscous fluid flows involving electrically charged particles and electric linear polarization and magnetization effects. All interaction between externally applied and internally induced electric and magnetic fields are incorporated in the model. We have also developed a fully conservative vector operator form of the EMHD system that is suitable for a direct discretization and numerical integration. Derivation of characteristic and non-reflecting open boundary conditions were also performed, thus completing the analytical part of the research effort. A numerical algorithm for iterative integration of the discretized fully conservative EMHD system in boundary-conforming non-orthogonal curvilinear coordinate system was developed that is based on dual time-stepping. Development of an accompanying computer code for the analysis of unsteady three-dimensional EMHD flows is in its final debugging stages.

Experimental measurements have been made in a cylindrical test cell containing liquid gallium. The cell is placed in the center of a rotating magnetic field and thermistors are used to measure temperature fluctuations. The stability of the system has been measured as a function of Rayleigh and Hartmann numbers. The application of a rotating magnetic field delays the onset of thermally-driven convection and increases the critical Rayleigh number. For weak rotating magnetic fields and small Hartmann numbers, the experimental observations can be explained by the existence of a single asymmetric roll rotating around the cylinder, driven by the azimuthal component of the magnetic field. The rotating magnetic field itself induces Reynolds instabilities for Hartmann numbers greater than approximately 3. The experiments indicate that a flow regime exists in which the benefits of a rotating magnetic field on the crystallization process are not compromised by time dependent flow.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 1
PhD Students: 0

TASK INITIATION: 9/94 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 962-21-08-24

NASA CONTRACT No.: NCC8-56

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:**Journals**

Volz, M.P., and Mazuruk, K. Flow transitions in a rotating magnetic field. Experiments in Fluids, vol. 20, 454-459 (1996).

Proceedings

Dulikravich, G.S., and Lynn, S.R. "Electro-Magneto-Hydrodynamics: Part 1 - Introductory Concepts." Symposium on Developments in Electro-Rheological Flows-1995, D.A. Siginer and G.S. Dulikravich, eds., ASME WAM '95, San Francisco, California, November 12-17, 1995, ASME FED-Vol. 235, MD-Vol. 71, pp 49-58.

Dulikravich, G.S., and Lynn, S.R. "Electro-Magneto-Hydrodynamics: Part 2 - A Survey of Mathematical Models." Symposium on Developments in Electro-Rheological Flows-1995, D.A. Siginer and G.S. Dulikravich, eds., ASME WAM '95, San Francisco, California, November 12-17, 1995, ASME FED-Vol. 235, MD-Vol. 71, pp 59-70.

Presentations

Dulikravich, G.S. "An unified theory of electro-magneto-gas dynamics." Hypersonics MAGLEV Group Meeting, National High Magnetic Field Laboratory, Tallahassee, Florida, December 1995.

Volz, M.P., and Mazuruk, K. "Damping of natural convection in liquid gallium with a rotating magnetic field." Tenth American Conference on Crystal Growth, Vail, Colorado, August 1996.

Models of Magnetic Damping for Semiconductor Crystal Growth in Microgravity

PRINCIPAL INVESTIGATOR: Dr. John S. Walker

University of Illinois, Urbana-Champaign

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective is to optimize the benefits of a magnetic field during semiconductor crystal growth in space. The tools for this optimization are models of the liquid motion and of the distribution of dopants or alloys, including the effects of a magnetic field. One potential benefit of a magnetic field is to reduce dramatically the adverse effects of the residual accelerations experienced by any experiment in an earth-orbiting vehicle. Another benefit is the elimination of the deleterious flow oscillations driven by surface tension in the floating-zone process. One major objective is to develop accurate methods to model the mass transport of dopants or alloys during crystal growth in space with a magnetic field.

Task Description:

This task includes three research projects:

1. Mass Transport of Dopants and Alloys during Crystal Growth in Space with a Magnetic Field.

Previous models assumed that the dopant/alloy distributions reach a steady state at each stage during crystal growth, but this assumption is not valid for crystal growth with a magnetic field. Modeling the actual transient mass transport accurately and with reasonable computational resources is the goal of this research. Our initial efforts are focused on thermally driven buoyant convection, but our models will be extended to include the compositionally driven buoyant convection in alloys.

2. Melt Motion Driven by Residual Accelerations.

The residual accelerations in any earth-orbiting vehicle consist of three components: (1) a steady or DC acceleration; (2) continuous and random fluctuations of acceleration; and, (3) isolated spikes of large acceleration. Models have been completed for the time-dependent three-dimensional melt motion driven by the fluctuations and spikes, and the model for the DC acceleration is nearly finished.

3. Magnetic Stabilization of Thermocapillary Convection during Floating Zone Crystal Growth in Space.

The floating-zone process avoids the problems arising from contact between the crystal and the ampoule wall, but it also involves surface-tension driven flows which are often unstable, even for very small temperature differences. The resultant oscillatory flows produce undesirable spatial variations of the dopant concentration in the crystal, called striations. A magnetic field can be used to stabilize the surface-tension driven motion and thus eliminate the striations in the crystal. Models are being developed to predict accurately the magnetic field strength needed to stabilize the flow and to predict the steady melt motion with magnetic stabilization.

Task Significance:

Future advances in computers and communications will depend on improvements in the quality of semiconductor crystals. The NASA program to grow semiconductor crystals in space will play a critically important role in the development of better crystals. Since ideal crystal growth is not achieved even in space, because of the accelerations of the space vehicle and certain flow instabilities which still occur in space, NASA is beginning to design a Magnetic Damping Furnace to use a magnetic field to eliminate these residual problems and to achieve the ideal crystal-growth process in space. The objective of our research is to develop models to guide the design of this Furnace in order to optimize the benefits of the magnetic field.

Progress During FY 1996:

From the beginning of our cooperative research agreement in May 1996 to the end of FY96, we made progress in three research areas:

1. Magnetic Damping of Melt Motions Driven by the Residual Accelerations of a Space Vehicle.

We completed models of the three-dimensional, unsteady melt motions driven by the time-dependent components of the residual acceleration. In our first model, we considered the periodic melt motion driven by the periodic component of the residual acceleration due to crew movement or machinery. We found that the motion due to the transverse component of the acceleration is much larger than that due to the axial component and that the motion driven by the low-frequency accelerations is much larger than the motion driven by the high-frequency ones.

We also completed a model of the transient decay of the motion after a spike of residual acceleration due to a thruster firing or the motion of a large mass such as the cargo-bay door. We found that the deleterious melt motion decays much faster with even a relatively weak magnetic field than it does without a magnetic field.

2. Mass Transport of Dopants.

We have completed an asymptotic model for the transient transport of a dopant during the growth of a crystal with a magnetic field. Unlike previous quasi-steady models, our model provides accurate predictions of the dopant distribution in the crystal based on the transient solution in the melt for the entire period of time needed to grow a crystal. We have also integrated the full equations and found that the error in the asymptotic solution is less than 5% for all magnetic flux densities above 0.5 Tesla.

3. Thermocapillary Convection in the Floating-Zone Process with an Axial Magnetic Field.

With a strong magnetic field, the thermocapillary convection is confined to a thin boundary layer adjacent to the free surface. We have completed a model for the strong circulation inside the thin free-surface layer including inertial effects and including the convective heat transfer due to this circulation. As the first step in a study of the magnetic suppression of the transition from steady to periodic thermocapillary convection, we investigated whether such transitions can occur with axisymmetric flows and found that they cannot. Future work will focus on unsteady, three-dimensional studies of instabilities, which are extremely computationally demanding. Therefore we have validated an asymptotic model which should provide a large reduction in the computational requirements. We found that the asymptotic model has an error of less than 1% for all Hartmann numbers above 200.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 4

TASK INITIATION: 5/96 **EXPIRATION:** 5/98

PROJECT IDENTIFICATION: 962-21-24

NASA CONTRACT NO.: NCC8-90

RESPONSIBLE CENTER: MSFC

Process-Property-Structure Relationships in Complex Oxide Melts

PRINCIPAL INVESTIGATOR: Dr. Richard Weber

Containerless Research, Inc.

CO-INVESTIGATORS:

Nordine, P.

Containerless Research, Inc.

Task Objective:

The research uses the control of chemistry and nucleation achieved by high temperature containerless liquid-phase processing to study non-equilibrium phase (glass) formation and crystal growth in oxide melts. The work is intended to advance the basic understanding of the high temperature chemistry and thermophysical properties of molten oxides. Non-contact measurements of melt temperature, viscosity, surface tension, and solidification velocity will be made and the results of these measurements will be used to interpret the materials behavior and to develop predictive models of solidification as a function of composition.

Task Description:

The effects of melt chemistry, temperature and processing variables, including gravity-driven convection on melt properties, solidification kinetics, metastable phase formation, and crystal growth, are being investigated. High temperature liquid-phase processing is by aeroacoustic or aerodynamic levitation in combination with continuous wave CO₂ laser beam heating. Levitated materials are observed by optical pyrometers, video cameras, and noncontact instruments to measure melt viscosity and surface tension. Processed materials are examined by optical and scanning electron microscopy, x-ray diffraction, nuclear magnetic resonance, Raman spectroscopy, and laser fluorescence techniques.

Task Significance:

The work provides insights into subtle chemical and transport effects on solidification and glass formation in complex oxide melts which mimic technologically and geologically important materials. The investigations explore the limits of ground-based measurement techniques and will identify systems which require the additional control of convective melt transport and liquid-liquid phase separation which may be achieved in extended-duration, reduced-gravity experiments.

Progress During FY 1996:

The FY96 research focussed on molten oxides selected from both a basic research and an applications development perspective. The effects of melt chemistry, temperature, and processing variables (including gravity-driven convection (sedimentation)), on melt properties, solidification kinetics, metastable phase formation, and crystal growth, are being investigated. High temperature liquid-phase processing is by aero-acoustic or aerodynamic levitation in combination with continuous wave CO₂ laser beam heating under controlled oxygen partial pressures.

Levitated materials are observed by optical pyrometers (i.e., video cameras). Non-contact instruments to measure melt viscosity and surface tension are being integrated with the levitation facility. Processed materials are examined by optical and scanning electron microscopy, x-ray diffraction, nuclear magnetic resonance, Raman spectroscopy, and laser fluorescence techniques.

Work has been focused on:

1. Review of recent literature on oxide properties.
2. Installation, testing and preliminary experiments using a high resolution video camera, frame grabber, and computer image analysis software.
3. Planning/design for integration of a Surface Fluctuation Spectrometer (SFS) instrument with the aero-acoustic levitator for measurements of melt surface tension and viscosity.

4. Conducted preliminary experiments on molten oxides with the $\text{Al}_6\text{Si}_2\text{O}_{13}$ (3:2 mullite), and $\text{Y}_3\text{Al}_3\text{O}_{12}$ (Yttrium Aluminum Garnet) compositions.

1. Phase diagrams for the alumina-silica, alumina-ytria, alumina-calcia, and alumina-zirconia systems have been reviewed. Recent literature on alumina-based binary materials was collected and reviewed.

The alumina-silica and alumina-ytria systems have been selected for investigation in the early part of the project and for use in experiments to develop the measurement techniques. The alumina-silica system was chosen because it combines the highly structured and viscous melt - silica - with an inviscid melt - alumina. The combination of alumina and silica provides melts with a wide range of viscosities to be made. The alumina-ytria system was selected because it has been shown to exhibit phase separation and oxygen-dependent solidification behavior.

2. A high resolution video camera and frame grabber was installed on the aero-acoustic levitator. The image of the levitated specimen fills approximately 50% of the active area of the CCD array. The images are acquired at a rate of 30 frames per second. Post processing image analysis is performed with a frame grabber and software which allows individual frames to be grabbed and analyzed. We have established that the melts are somewhat transparent at near infrared wavelengths where the camera is most sensitive. The melt transparency allows in-situ observation of crystal growth and fluid motion.

3. A kick-off meeting was held at NASA Lewis to determine requirements for integration of the SFS instrument with the aero-acoustic levitator. Ray traces show that the 0.3 cm diameter specimen will act as a powerful lens and cause the probe beam to diverge. The requirements for the imaging system to collect light reflected from the specimen are being investigated.

4. Experiments on solidification of melts with the composition $\text{Al}_6\text{Si}_2\text{O}_{13}$ (3:2 mullite) composition show that: (i) in argon, the liquid can be undercooled by approximately 300 °C before spontaneous recrystallization (recalescence) occurs to form an opaque white solid; and (ii) in oxygen, recalescence is not observed and transparent specimens are formed. Analysis of high resolution video images of materials processed in argon show that the growth front moves across the specimen at a rate of ca. 0.1 cm s^{-1} .

Materials with the $\text{Y}_3\text{Al}_3\text{O}_{12}$ (Yttrium Aluminum Garnet) composition show a strong oxygen pressure dependence on the solidification behavior. Melts equilibrated with pure oxygen do not resolidify, but cool continuously to form an amorphous material. Melts processed in argon recrystallize to form material with the isometric garnet structure when indexed by x-ray diffraction. Specimens of crystalline and amorphous materials are being investigated by high temperature reaction calorimetry through a collaboration with Professor Navrotsky at Princeton University. The calorimetric results will establish the relative thermodynamic stability of the amorphous and crystalline phases.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 6/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 962-21-32

NASA CONTRACT NO.: NAS8-408

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Biswas, A.B., Weber, J.K.R., and Nordine, P.C. Cr^{3+} Fluorescence in Containerless Melt-purified Aluminum Oxide. J. Mat. Res., vol. 10, 1823-1827 (1995).

Weber, J.K.R., and Nordine, P.C. Containerless Liquid-Phase Processing at High temperatures. Microgravity Science and Technology, vol. VII, 279-282 (1995).

Weber, J.K.R., Anderson, C.D., Krishnan, S., and Nordine, P.C. Structure of Aluminum Oxide Formed from Undercooled Melts. J. Am. Ceram. Soc., vol. 78, 577-582 (1995).

Weber, J.K.R., Felten, J.J., and Nordine, P.C. New Method for High Purity Ceramic Synthesis. Rev. Sci. Instrum., vol. 67, 522-524 (1996).

Weber, J.K.R., Felten, J.J., Cho, B., and Nordine, P.C. Design and Performance of the Aero-Acoustic Levitator. J. Jpn. Soc. Microgravity Appl., vol. 13, 27-35 (1996).

Weber, J.K.R., Krishnan, S., and Nordine, P.C. Effects of Melt Chemistry on the Spectral Absorption Coefficient of Liquid Aluminum Oxide. J. Am. Ceram. Soc., vol. 78, 3067-3071 (1995).

Proceedings

Weber, J.K.R. "Containerless Property Measurements on Molten Aluminum Oxide and Alumino-Silicate Binary Mixtures." Proc. 4th Asian Thermophysical Properties Conference, Tokyo, Japan, September 5-8, 1995, A. Nagashima, ed., pp 873-876.

Presentations

Weber, J.K.R. "From Basic Research to Applied Materials - Containerless Liquid-Phase Processing of Molten Oxides." Department of Materials Science Research Seminar, University of Illinois at Urbana-Champaign, Champaign, Illinois, September 19, 1996.

Weber, J.K.R., and Nordine, P.C. "Process-Property-Structure Relationships in Complex Oxide Melts." NASA Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Weber, J.K.R., Felten, J.J., Cho, B., Lockwood, N., and Nordine, P.C. "New Observations of Undercooled Oxide Solidification." Gordon Research Conference on High Temperature Chemistry, Tilton School, Tilton, New Hampshire, July 23, 1996.

Thin Film Mediated Phase Change Phenomena: Crystallization, Evaporation and Wetting

PRINCIPAL INVESTIGATOR: Prof. John S. Wettlaufer

University of Washington

CO-INVESTIGATORS:

Elbaum, M.
Stone, H.A.
Worster, M.G.Weizmann Institute of Science
Harvard University
University of Cambridge (Great Britain)

Task Objective:

Our objective focuses on experimental and theoretical studies of volatile thin liquid films that originate in two distinct physical settings, but which are linked by similar theoretical descriptions. The films are either (i) deposited on a substrate via direct adsorption from the vapor or (ii), formed at the interface between a solid and its vapor through the process of surface melting. The relevance to microgravity materials research lies in the fact that during wetting, drying, and spreading the configurations of fluid-solid interfaces control nucleation processes and directly affect heat and mass transfer rates. During Czochralski growth, laser welding, float-zone processing, nucleation on or near substrates, Ostwald ripening, physical vapor transport, and sintering, the shape of fluid-solid and fluid-vapor interfaces can control material structure and properties. Cohesion and adhesion of thin films in microgravity is dominated by intermolecular interactions and interfacial tensions, and inertial effects that are independent of gravity can control thin film dynamics in space. As the capillary length is extended, the thin film phenomenon we observe on earth may extend to much larger scales in space. Therefore, earth-based thin-film studies offer an ideal test bed for the phenomena that dominate space-based processes.

Task Description:

We will investigate liquid films on inert substrates and liquid films on crystal surfaces. In the first area we will study the dynamical mechanisms associated with heterogeneous dewetting processes, and the frustration or enhancement of nucleation in proximity of the substrate. Experiments will use systems designed by Prof. Elbaum. They will quantify the relation between the driving force and the spreading/dewetting rates and the role of long range interactions in nucleation in proximity to walls. They will search for crossovers in which long range interactions give way to gravity. Theory seeks to determine the origin of the observed instabilities so we can extend understanding to other vapor/liquid/substrate systems. We will also study the dynamics of the crystallization and evaporation when solutes are present in the film and the variation in nucleation rates due to proximity effects. In the second area we will investigate the transport of films at the crystal/vapor interface that form through the process of surface melting. This will be primarily theoretical.

Task Significance:

The focus of our research is important because the processes we intend to unravel have significant implications for fluid containment or transport in space. Furthermore, since evaporation and condensation processes are continually encountered when handling liquids on earth we expect them to play a significant role in future terrestrial applications. Uniformity and composition of thin-film coatings, crucial to our nation's technological development, will depend on the processes we are studying. Our research focuses on overcoming major obstacles to the growth of uniform crystals. These interfacial phenomena have implications for fuel handling, welding, brazing, soldering, ceramics and electronics industries, and other practical materials processing situations.

Progress During FY 1996:

Our project began in May of 1996. Hence, progress during the last few months has been limited to (a) design and preliminary construction of the experimental apparatus and (b) the carrying out of a stability calculation relevant to one of the task objectives: the crystallization and evaporation of thin films when solutes are present. The latter is being refined and will be written up for publication during FY96.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 **EXPIRATION:** 4/97

PROJECT IDENTIFICATION: 962-21-08

NASA CONTRACT No.: NAG8-127

RESPONSIBLE CENTER: MSFC

Defect Generation in CVT Grown $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ Epitaxial Layers under Normal and Reduced Gravity Conditions

PRINCIPAL INVESTIGATOR: Dr. Heribert Wiedemeier

Rensselaer Polytechnic Institute

CO-INVESTIGATORS:No Co-I's Assigned to this Task

Task Objective:

The generation and propagation of defects are very complex phenomena in heteroepitaxial layer growth.

The primary objectives of this task are to differentiate between the effects of gravity-driven convection and of inherent properties of the layer/substrate assembly on the formation of defects. The inherent parameters include lattice mismatch, substrate orientation and surface state, and growth rate.

Task Description:

Epitaxial layers of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ will be grown on substrates in closed, fused silica containers by chemical vapor transport. For this purpose, different substrates, crystallographic orientations and surface defect density, as well as different temperature profiles, will be employed.

Identical experiments will be performed under vertical, stabilizing and horizontal orientations of the density gradient relative to the gravity vector in order to elucidate the effects of convective flow on the layer morphology and properties for different, inherent parameters.

Task Significance:

Our experiments are expected to provide valuable insight into the complex interrelations between fluid flow and other experimental parameters. The observed trends represent useful information for the further development of meaningful models of epitaxial growth.

Because of the importance of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ and related systems for device applications, these studies are of basic scientific and technological significance.

Progress During FY 1996:

The primary objectives of this task are to differentiate between the effects of gravity-driven convection and of inherent properties of the layer/substrate assembly on the formation of defects. An important inherent parameter is the crystallographic relationship between the substrate and the epitaxial layer to be grown on the substrate.

Epitaxial growth experiments are in progress to investigate the effects of off-orientation of the CdTe substrate from the nominal (100) orientation on the growth properties of the epitaxial layers. Initial observations indicate measurable effects of small deviations from the (100) substrate orientation on the morphology of the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ layer surface and of the $\text{Hg}_{1-x}\text{Cd}_x\text{Te}/(100)\text{CdTe}$ layer/substrate interface.

These investigations are continued and extended to different substrate orientations.

STUDENTS FUNDED UNDER RESEARCH:**TASK INITIATION:** 6/96 **EXPIRATION:** 5/98**PROJECT IDENTIFICATION:** 962-21-25**NASA CONTRACT No.:** NAG8-126**RESPONSIBLE CENTER:** MSFC

Use of Microgravity to Control the Microstructure of Eutectics

PRINCIPAL INVESTIGATOR: Dr. William R. Wilcox

Clarkson University

CO-INVESTIGATORS:

Regel, L.L.
Smith, R.W.Clarkson University
Queens University**Task Objective:**

This project began in June 1996. The long term goal is to be able to control the microstructure of directionally solidified eutectic alloys through an improved understanding of the influence of convection. The primary objective of the present project is to test hypotheses for the observed influence of convection on the microstructure of three fibrous eutectics (MnBi-Bi, InSb-NiSb, Al₃Ni-Al). A secondary objective is to determine the influence of convection on the microstructure of other eutectic alloys.

Task Description:

Prior experimental results on the influence of microgravity on the microstructure of fibrous eutectics have been contradictory. Theoretical work at Clarkson University showed that buoyancy-driven convection in the vertical Bridgman configuration is not vigorous enough to alter the concentration field in front of a growing eutectic sufficiently to cause a measurable change in microstructure. Currently, there are three hypotheses that might explain the observed changes in microstructure of fibrous eutectics caused by convection:

1. A fluctuating freezing rate, combined with unequal kinetics for fiber termination and branching.
2. Off-eutectic composition.
3. Presence of a strong habit modifying impurity.

We favor the first of these hypotheses. We performed ground-based experiments using electric current pulses to deliberately create an oscillatory freezing rate. Although current pulsing coarsened the microstructure of MnBi-Bi eutectic as predicted, it may also have introduced localized convection. Current pulsing experiments in microgravity are needed to fully test this hypothesis.

Experimental and theoretical research will be carried out in collaboration with Professor Reginald Smith of Queens University. Through the support of the Canadian Space Agency, he has two automated furnaces located in the Canadian Microgravity Isolation Mount (MIM), in Prioroda on *Mir*.

Task Significance:

Solidification of eutectic alloys in microgravity has produced more regular microstructures. In the case of fibrous eutectics, the microstructure has also been quantitatively different. Thus microgravity research has demonstrated the potential to produce superior materials, both in space via reduced convection and on earth via improved understanding of convective effects. This task will enable reproducible production of superior eutectic alloys utilizing microgravity.

Progress During FY 1996:

A doctoral student was recruited in July. She has read the relevant literature, acquired and checked out equipment and supplies for experiments in our laboratory, and prepared growth ampoules. A continuing dialog with Professor Smith has been carried out to determine the alloys to be solidified aboard *Mir*. Another doctoral student has been recruited for the theoretical modeling, and he will begin in January, 1997.

STUDENTS FUNDED UNDER RESEARCH:BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 5/96 EXPIRATION: 4/00

PROJECT IDENTIFICATION: 962-21-09

NASA CONTRACT NO.: NAG8-126

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Wilcox, W.R., and Regel, L.L. "Influence of Convection on the Microstructure of Fibrous Eutectics." American Conference on Crystal Growth - 10, Vail, Colorado, July 1996.

Wilcox, W.R., Regel, L.L., and Smith, R.W. "Use of Microgravity to Control the Microstructure of Eutectics." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

BSO/BTO Identification of Gravity Related Effects on Crystal Growth, Segregation, and Defect Formation

PRINCIPAL INVESTIGATOR: Dr. August F. Witt

Massachusetts Institute of Technology (MIT)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Knowledge gained from space experiments and the related ground-based program is expected to advance the science base for crystal growth of oxides and thus to narrow the still existing gap between theory and experiment. More specifically, the proposed program provides an approach to the deconvolution of the effects of largely uncontrolled, complex processing variables on crystal growth and segregation, leading to the identification of growth conditions by which device specific property requirements in oxides can be approached. Such growth conditions are expected to be realizable in a modified Bridgman growth geometry, the subject of development in the ground-based support program.

Task Description:

The on-going research program on growth and characterization of BSO places the focus on a class of materials (optical and opto-electronic) with theoretical properties that are outstanding, but which have so far failed to reach their potential primarily because of our inability during growth to adequately control their stoichiometry, incorporation of functional minority constituents, crystal defect formation and confinement related contamination. Theoretical considerations indicate that the majority of existing growth deficiencies, which are responsible for our inability to produce viable device structures, are directly or indirectly related to gravitational effects. Thus it appears that an assessment of the true potential of selenites, which exhibit outstanding piezoelectric properties and exceptionally light optical rotative activity in device application, can at this time best be made on material obtained from controlled growth experiments in a reduced gravity environment. Under such conditions convective interference, otherwise unavoidable, is projected to be substantially suppressed and defect structures resulting during growth are expected to approach equilibrium values. Magnetic melt stabilization, found effective in growth of semiconductors, is ineffective in oxide systems.

Task Significance:

The research to date has focused on (a) the development of BSO single crystal growth capability by the Czochralski technique, (b) the characterization of growth and defect formation in BSO, and (c) the development of a Bridgman-type growth configuration for BSO that permits enhanced heat transfer control under quantifiable thermal boundary conditions and which is functionally compatible with NASA-generated existing hardware. The establishment of quantifiable growth conditions and the *in situ* growth characterization capability by means of current induced interface demarcation are considered essential in efforts directed at assessing the potential of reduced gravity environment for crystal growth research and development since the customary empirical approach is considered prohibitive in space experimentation. The approach taken is in addition also considered a key element in efforts to establish advanced crystal growth capabilities on earth, a prerequisite for the meaningful assessment of the potential of selenites in device applications.

Progress During FY 1996:

The growth characteristics of a three-zone vertical Bridgman-Stockbarger system with axial gradient control were investigated using Ga doped Ge as a model system. Stabilization of the growth interface location was approached by fixation of the axial temperature gradient through positioning the temperature control sensors for the high and low temperature heat pipes in the gradient region. Growth experiments were carried out with current induced interface demarcation. Thus, in post-growth analyses, the location and morphology of the crystal melt interface as well as the microscopic rate of growth during all stages of growth could be determined. The related segregation behavior was extracted from single point speeding resistance measurements. The results obtained and general conclusions on growth control in vertical Bridgman geometry have been submitted for publication.

Thermal characterization of the gradient zone revealed radial temperature asymmetries which could be attributed to the installation of monitoring temperature sensors. Elimination of this interference and elimination of heat losses at the junction heatpipe-gradient zone is pursued through a redesign of the gradient zone and the use of hollow micro-spheres (quartz, 0.3 mm diameter) as insulation matrix.

The scale of planned growth experiments has been extended to include the system BGSO (Bismuth silicate-germanate). The growth behavior of this system is first to be tested by means of the Czochralski technique.

STUDENTS FUNDED UNDER RESEARCH:

BS Students:	0	BS Degrees:	0
MS Students:	0	MS Degrees:	0
PhD Students:	2	PhD Degrees:	1

TASK INITIATION: 1/93 EXPIRATION: 1/96

PROJECT IDENTIFICATION: 962-21-08-19

NASA CONTRACT No.: NAG8-949

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Becla, P., Witt, A.F., Lagowski, J., and Walukiewicz, W. Large photo-induced persistent optical absorption in Se doped AlSb. Appl. Phys. Lett., 67, (3), 395-397 (1995).

Lin, C. and Witt, A.F. New approaches to growth and characterization of photo-refractive BSO (B12SiO20). J. Crystal Growth, (accepted, 1996).

Papa Rao, S.S. and Witt, A.F. Control of growth interface location and morphology in a heatpipe-based vertical Bridgman system. J. Crystal Growth, (accepted, 1996).

Presentations

Witt, A.F. and Presinger, A. "An initiative for European collaboration in crystal growth research and technology development." BMFW, Vienna, Austria (1995).

Thesis

Papa Rao, S.S. Control of the growth interface location in vertical Bridgman geometry (PhD Thesis, MIT). (1996).

Free Float Trajectory Management ATD

PRINCIPAL INVESTIGATOR: Mr. A. P. Allan

University of Delaware

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

Many researchers perform experiments that are sensitive to the effects of gravity aboard aircraft flying low gravity trajectories. The aircraft is flown in a ballistic trajectory during which a period of free-fall is attained, providing the desired low gravity environment. These trajectories are characterized by an initial trajectory entry phase which can be very dynamic, followed by the stabilized low-g period and finally, an exit phase. Ideally, the entry phase should be minimized to allow the longest possible low-g time.

The low-g environment experienced by an experiment attached to the aircraft is degraded by vibrations from the aircraft as well as directly imposed disturbances from acoustics, air flow, or that are self-induced. However, an experiment package allowed to free-float during the stabilized low-g phase will only be affected by the direct disturbances which are usually inconsequential for most experiments. The drawback of free-floating an experiment is that the package typically contacts the walls of the aircraft after only a few seconds due to the initial velocity of the package at release and the rotation of the aircraft during the parabolic trajectory. Longer free-float times are achievable, but are not predictably reproducible.

The objective of this work is to develop the technology for an extended, consistently reproducible acceleration environment during the stabilized low-g phase of the trajectory, specifically for free-float packages. The goal is to extend the free-float time to 10 seconds or longer and obtain stable accelerations of 0.001 g or lower in a consistent, reproducible manner.

Task Description:

Improving the low-g environment for free-float packages requires the optimal control of the aircraft trajectory and the release of the package. The control of the trajectory is dependent on the limitations of the specific aircraft used and the feedback the pilots use to maneuver through the trajectory. The definition of the trajectory in terms of air speed and pitch angle when entering the trajectory, the acceleration level during pull-up, and the air speed and pitch angle when exiting the trajectory is the first step in maximizing the overall trajectory time and, in particular, the stable low-g time.

To control the aircraft maneuver during the low-g phase, specific commands for pitch, roll and throttle must be provided to the pilots. This requires the development of a control law to develop the appropriate commands. The control law is based on the states of the aircraft and the position of the experiment package in the aircraft cabin.

The controlled release of the experiment package once the stable low-g environment has been established will provide a consistent means of initializing the free-float period. By optimizing the initial release velocity, the package will rise off the aircraft floor and the controller will monitor its location in the aircraft. The control law will develop the appropriate control commands for the pilots to essentially fly the aircraft about the trajectory of the free-floating package. The control commands will be displayed to the pilots graphically.

The test bed for the developed technology will be the NASA LeRC DC-9 aircraft.

Task Significance:

By providing a facility that can produce consistent results as described above, more experimenters will benefit from longer duration and better quality low-gravity testing. Experimenters will be able to count on a good trajectory every time rather than working on a trial-and-error basis. Some programs could conceivably be done completely on the DC-9 without having to go to suborbital or spaceflight carriers.

II. MSAD Program Tasks — Advanced Technology Development

Progress During FY 1996:

In FY 1996, initial flight testing was performed to obtain baseline data on the current performance of the DC-9 and the quality of the trajectories. Typically, free-float trajectories have acceleration levels of less than 0.001 g and last approximately 4 seconds. Out of nearly 1000 trajectories, less than 5 lasted 10 to 11 seconds.

A rack release system was developed to push the rack off the aircraft cabin floor once a stable low-g environment is attained. The rack is held in place by electromagnets during the pull-up portion of the trajectory. Once the stable low-g is attained, the electromagnets are turned off and the rack is pushed away by four small pneumatic cylinders. Flight testing of this system was performed in June.

A three dimensional positioning system for tracking the location of the rack during free-float was added to the system. The system uses blinking infrared LEDs that are tracked by a set of 3 linear-array CCD cameras. The location of 7 LEDs mounted on the free-floating rack is determined in realtime and then transferred to the control computer. The control computer selects the most optimal set of 3 LEDs observed by the camera to calculate the location of the rack in three-dimensional space. This information will be used in the implementation of the trajectory guidance system. Flight testing of the position tracking system was performed in August.

Instrumentation of the DC-9 aircraft to measure aircraft control surface positions and pilot inputs continues whenever the aircraft is available. This data is necessary for the implementation of the trajectory guidance system. Testing of the instrumentation and aircraft parameter identification flight testing is planned for the Fall of 1996.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/94 EXPIRATION: 9/97

PROJECT IDENTIFICATION:

NASA CONTRACT No.: NCC3-429

RESPONSIBLE CENTER: LeRC

II. MSAD Program Tasks — Advanced Technology Development

Low Temperature Magnetostrictive Smart Actuator Mechanisms

PRINCIPAL INVESTIGATOR: Dr. Robert G. Chave

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Barmatz, M.

Fultz, B.

Hahn, I.

Jet Propulsion Laboratory (JPL)

California Institute of Technology

Jet Propulsion Laboratory (JPL)

Task Objective:

The objective of this project is to use the unique "giant" magnetostrictive properties of terbium, dysprosium and zinc alloys as the prime mover in a series of actuators and mechanisms which include low temperature valves, heat switches precision positioners, and lead screw drivers. These new materials have performance characteristics for low temperature operation hitherto unavailable in any actuator. We are developing these materials and a family of devices for use at low temperature based on their unique properties of long stroke and high power with negligible energy dissipation.

Task Description:

The four-year task consists of a program of a low temperature materials test facility development, development of the materials themselves, development of material applications, and a program of field testing of the devices produced under the program.

The facility development is centered around the generation of a dewar with a fringe counting interferometer, and a interferometric vibrometer, plus a Hall effect sensor and integrating magnetometer for measuring variations in the displacement vs. applied field in the test materials. Materials development is focused on increasing the performance, easing the manufacturability, and reducing the hysteresis present in some variants of the material. The applications of special interest are liquid helium valves, including superfluid helium valves, and other low temperature actuated devices such as heat switches and precision positioners which are of utility to PI's in the Code UG program and in NASA generally. The final phase is a program of field testing in which the prototypes produced by this task will be independently evaluated by Code UG PI's and others in the field.

Task Significance:

Because of the extraordinary strokes which are available from these crystals, a level of effectiveness is being realized in these devices which was previously unavailable in the world of cryogenic instrumentation. By comparison, the piezoelectric effect, when used at helium temperature, produces a stroke which is approximately 80 times smaller per unit length of actuator crystal. This difference is enhanced in that the usable lengths of single crystals of terbium dysprosium are longer than those of available piezoelectric crystals.

Generally, physical effects tend to be attenuated with reduced temperature. Electrostriction and piezoelectric actuation are greatly reduced in effectiveness. By contrast, the magnetostrictive effect is actually enhanced at low temperatures, and the greatest power and longest strokes are available around helium temperature. Coincidentally, this is the temperature range in which superconductive solenoids are most easily applied to excite the magnetostrictive effect. The fabrication of helium valves is greatly eased by these physical properties because the temperature of the prime mover is then optimally maintained at that of the working fluid in the valve. All forces may be reacted locally, and heat leaks to the external surface of the dewar are completely eliminated. The first magnetostrictive helium valves were produced by the Co-Investigators of this program, using these materials, and others are in development. Other devices requiring a truly cold prime mover, with minimum heat dissipation, such as heat switches will also be developed.

Progress During FY 1996:

During fiscal year 1996 a major thrust was the design, construction and test of a facility for measuring the magnetostrictive effect at helium temperatures. A dewar was obtained with a large-volume (30 liters) helium cold finger, and a still larger vacuum space above the cold finger. This dewar has optical access along the centerline of

II. MSAD Program Tasks — Advanced Technology Development

the dewar, through the radiation shields, for the beam path of an interferometer. A fringe-counting interferometer for measuring linear displacements was obtained and installed. An interferometric laser vibrometer for measurement of linear displacement with 8 nanometer resolution in sub-millisecond time intervals was also obtained (as surplus from another project) and was characterized. Various approaches to Hall effect measurement of the magnetic field in and around the sample have been tried, and this problem is now believed to be solved. An integrating, magnetometer using a coil around the sample has also been built. This entire facility has largely been characterized at helium temperature, and sample development tests are now commencing.

In the material development area, six samples of terbium dysprosium were obtained from the Materials Preparation Center, a DOE facility in Ames, Iowa, and are scheduled for various applications. A new type of terbium dysprosium and zinc, which can be grown using the less-expensive Bridgeman method, was designed by A. E. Clark, and testing is pending. This material has the desirable property that it can be machined, drilled and tapped, where previous formulations could not be. Full characterization tests are pending. The possibility of using polycrystalline versions of terbium dysprosium actuators was reviewed by Brent Fultz of Caltech's Materials Science Department, who recently joined the task as a co-investigator. He and Marius Birsan, a postdoc supported partially by this effort, are developing a method of obtaining the desired crystalline orientation primarily by pressing and rolling the material through a rolling mill. This approach, if achieved, has the potential to reduce the cost of these materials very significantly.

Valve designs for liquid helium were studied and review. Microscope study photographs of failed valve plungers and seats were produced and examined. A career valve designer with extensive NASA and space flight experience was located and hired as a consultant to the project. One valve with reduced dead volume was attempted with moderate success. Detail drawings of an improved helium valve with minimal dead volume have been generated, and the valve will be fabricated soon. This valve will be available for beta-site testing this Summer.

In the area of linear actuators a room temperature version of a very high resolution, long travel linear positioner have been produced. This is the first such magnetostrictively based, high resolution, long travel reaction mass motor. The motor has 50 nanometer resolution, in present versions, and travel which is unlimited except by the length of the rails along which the positioner slide. A low temperature version is contemplated, which will be the first such low temperature linear motor. Low temperature applications are expected to be easier than the room temperature one, given the higher performance of magnetostrictive materials at low temperature. A zero-gravity, three-axis version is also under consideration, which will be the first three-axis type. JPL New Technology Reports (NTR) for these developments are in various stages of preparation. A room temperature version of a lead screw driver for low temperature application, with all-rolling contact and high axial stiffness, was designed and a NTR submitted.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/95 EXPIRATION: 9/99

PROJECT IDENTIFICATION:

RESPONSIBLE CENTER: JPL

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

NASA Tech Briefs

Chave, R.G. Magnetostrictive Lead Screw Driver for Optics Positioning at Liquid Helium Temperature. NASA Tech Brief, JPL New Technology Report, (1996).

Presentations

Chave, R.G., Wiseman, T.A.J., Barmatz, M.B., and Hahn, I. "A Facility for Interferometric Measurement of Linear Displacement in Actuators and Calibration of Sensors at Cryogenic Temperatures Between 4.2 K and 77 K." SPIE 2865-10, SPIE Annual Meeting, Denver, 1996.

Fultz, R., Chave, R.G., Birsan, M., and Barmatz, M.B. "New Polycrystalline Materials for Low Temperature Actuators in Space Science Instruments." Proposal to the President's Discretionary Fund Caltech, 1996.

II. MSAD Program Tasks — Advanced Technology Development

Real-Time X-Ray Microscopy for Solidification Processing

PRINCIPAL INVESTIGATOR: Dr. Peter A. Curreri

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Kaukler, W.

University of Alabama, Huntsville (UAH)

Task Objective:

The objective of this ATD consists in the development of an X-ray Transmission Microscope (XTM) for the *in situ* and real-time observation of interfacial processes in metallic systems during freezing or solid-solid transformation. The XTM should have the following capabilities:

1. Provide a resolution for specimen features of 10-100 μm ;
2. At solidification rates of 0.1 to 20 $\mu\text{m}/\text{sec}$;
3. Temperatures up to 1100 $^{\circ}\text{C}$ with temperature gradients up to 50 $^{\circ}\text{C}/\text{cm}$;
4. With contrast sensitivities sufficient to detect 2-5% difference in absorptance;
5. Offer 1, 2, and 4 in exposure times of a few seconds; and,
6. Permit recording of stereo pairs for depth information.

Task Description:

The purpose of this ATD is the development of a high resolution x-ray either during freezing or solid-solid transformations. We will use the X-ray Transmission Microscope (XTM) to view, *in situ* and in real-time, interfacial processes in metallic systems. XTM will operate in the hard x-ray range (10 to 100 KeV) and achieve magnification through projection.

Task Significance:

Physical processes which occur at, or near, interphase boundaries during solidification, or other phase transformations, play a major role in the determination of many of the technologically important properties of solids. To date, interfacial morphologies and particle-interface interactions in the respective metallic, optically opaque systems have been deduced from post-process metallographic analyses of specimens. Thus, little information is obtained about the detailed dynamics of the processes. These investigations have been considerably augmented by real-time observations of transparent materials; yet, since some of the interfacial and transport properties of these materials differ greatly from those of metals and semiconductors the results are not necessarily representative of these opaque systems.

Progress During FY 1996:

The main efforts were the construction of the x-ray furnace, evaluation and selection of the technology for the advanced x-ray camera, the establishment of criteria for and selection of peripheral equipment, solidification experiments with Al alloys and Al-Zirconia composites in the prototype furnace, evaluation of the specimens for the "Particle Pushing at Interfaces" flight definition experiment (Dr. Stefanescu, University of Alabama, PI), measurements of emitted spectra from x-ray source, and testing of higher resolution x-ray targets.

The goals of the project objectives have been met. Cellular structures have been observed during solidification of Al-Ag alloys with dimensions of 50 micrometers width or less. Imaging of solidifying interface with growth rates of 0.2 $\mu\text{m}/\text{sec}$ to 34 $\mu\text{m}/\text{sec}$ has been demonstrated. A 3.5% contrast sensitivity was achieved using the high definition x-ray source and detection system with large features.

Four technologies, all based on CCD's, were evaluated for the advanced x-ray camera/converter. A cooled CCD with a fiber optic faceplate and a CsI phosphor material 1242-by-1152 pixels and 16-bit gray scale resolution was found to provide the optimum performance.

An advanced x-ray transparent furnace has been designed and is being constructed. The prototype furnace enables a maximum real-time magnification of a solidifying sample of about 50 X. The advanced furnace is designed to allow a magnification of 200 X, which could allow real-time imaging of growth of fine microstructural features (such as fibers in eutectic and monotectics) in these opaque metallic alloys for the first time.

II. MSAD Program Tasks — Advanced Technology Development

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/94 EXPIRATION: 10/96

PROJECT IDENTIFICATION: 963-70-04

RESPONSIBLE CENTER: MSFC

Single Electron Transistor (SET)

PRINCIPAL INVESTIGATOR: Dr. Pierre Echternach

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

LeDuc, H.G.

Jet Propulsion Laboratory (JPL)

Maker, P.D.

Jet Propulsion Laboratory (JPL)

Bozler, H.

University of Southern California

Task Objective:

The objective of the proposed effort is to develop an electrometer (Single Electron Transistor) capable of a resolution of $10^{-6} e/Hz^{1/2}$, where e is the electron charge, operating at 4.2K using Nb/Al₂O₃/Nb technology.

Task Description:

A mesoscopic single electron transistor (SET) is formed from two tunnel junctions whose capacitances are small, of the order of 10^{-15} Farad or smaller. The common electrode is capacitively coupled to the source of the charges to be measured. Changes in the capacitively coupled charge by fractions of a single electron charge will modulate the current passing through the junctions. The main technological problem is fabrication of the junctions. The junctions will be formed using e-beam lithography. The technological basis is developed in JPL's Microdevices Laboratory.

This task will result in a design for the charge amplifier that will take into account the feasibility of the processing steps involved in it, such as the limits of electron-beam lithography and the verticality of etch during the reactive ion etching steps, for example. By employing smaller and smaller aluminum-based junctions as described below in the Progress section, the devices fabricated will be tested first at subkelvin temperatures, and eventually expecting SET performance at 4.2 K from the smallest junctions. The success criteria of the task will be obtaining devices with satisfactory current-voltage characteristics at these easily accessed temperatures.

Task Significance:

Development of technologies required for production of a SET will allow making working SET in the next task's period. This in turn will open new possibilities for controlling and reading out different experimental variables. SET is suitable for measuring many parameters of the materials under investigation. Examples include measurements of dielectric constant, pressure, density, temperature, charge, voltage, etc. The parameters whose measurement can be reduced to capacitance measurements are especially suitable for measurements with SET. Unlimited dynamic range of SET allows precise measurements even in cases when a capacitive method with present techniques does not lead to sufficient sensitivity.

For example, it is feasible that SET-based thermometers will have resolution comparable to or exceeding that of High-Resolution Thermometers, presently used in several flight experiments, designed or supported by JPL. In addition, SET is compact in size. This small size will allow miniaturization of SET-based devices and creating arrays of them, accelerating information collection and in many cases decreasing flight time required to conclude an experiment. Miniaturization of the experiments is also very much in line with JPL's goal of creating miniature spacecraft.

Progress During FY 1996:

Last year we described two different approaches to the design that we were trying. The first approach is based directly on miniaturization of the technology already existent at the Microdevices Laboratory for fabrication of small tunnel junctions. The second approach is a departure from the "traditional method" and involves a different technology of making junctions called "edge junctions." Each method has its advantages and disadvantages. In each approach roughly three designs were tried, each solving problems encountered in the previous version.

The tests of the current-voltage (I-V) characteristics of the devices fabricated which were performed at JPL this year. The devices fabricated using the "edge" method that showed good I-V characteristics at 4.2K were tested at dilution

refrigeration temperatures. No charge amplification behavior was observed in any of them so far. We suspect that heating caused by bias currents in the junctions keeps the junctions from cooling, so it wipes out the expected step behavior at low temperatures.

To avoid these heating effects, we intend to stop using niobium, which is difficult to make in very small-area junctions, and start using aluminum, where fabrication problems will be greatly reduced. New masks have been designed and fabricated. New junctions will be made with these masks from aluminum, and these new junctions will be tested at subkelvin temperatures where the step behavior is expected. Then the size of these junctions will be reduced in a series of steps to allow them to show the SET behavior at higher and higher temperatures.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 10/94 **EXPIRATION:** 10/95

PROJECT IDENTIFICATION: 963-01-04-02

RESPONSIBLE CENTER: JPL

II. MSAD Program Tasks — Advanced Technology Development

Advanced Heat Pipe Technology for Furnace Element Design

PRINCIPAL INVESTIGATOR: Dr. Donald C. Gillies

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Palosz, W.

USRA/NASA Marshall Space Flight Center (MSFC)

Task Objective:

This project is aimed at an important advance in the fabrication of heat pipes and incorporating them into existing furnace technology. The main task is to fabricate a heat pipe to operate as an isothermal furnace liner capable of processing materials at temperatures up to 1500 °C. The isothermality and control associated with a heat pipe greatly exceeds that possible in traditional wire wound furnaces, and thus improves the quality of the thermal environment. Existing technology for isothermal liners limits the application to 1100 °C, and the extension to the higher temperature range will enable materials science experiments to be controlled with more favorable thermal conditions. Experiments contemplated for the higher range include crystal growth by solidification of high temperature materials such as cadmium telluride and gallium arsenide, and application to other advanced fabrication techniques such as liquid phase sintering. The measurement of thermophysical properties such as diffusion constants of dopants and thermal diffusivity in liquid semiconductors, including silicon, at well controlled temperatures is another important application.

The isothermal furnace liner is aimed at installation within a module on the Space Station Furnace Facility on the International Space Station, but has immediate application to ground-based studies, where tight control of temperature will be beneficial. The second part of this ATD project is to breadboard the equipment and to determine the protocol for incorporating the hardware into future missions. In a man-tended environment, the presence of reactive liquid metals at high temperatures will demand the use of adequate containment procedures and strict protocol for the handling of the high temperature components to ensure the safety of the crew members.

Task Description:

A major part of the high temperature heat pipe is the need for selecting the materials for its successful fabrication. One of the main efforts has been to review the possible materials, and to examine their known history as conventional heat pipes. An extensive range of materials was considered to determine the most appropriate cost effective approach for use in this project. A clear decision was made to use lithium as the working fluid. With a low melting point (181 °C) and vapor pressure just below atmospheric at the required operating temperature, its properties are ideal. Furthermore, there is an adequate data base of its use in the past for heat transfer applications within this temperature range. Purification and loading techniques of lithium for heat pipe applications are well understood and the technology is at a mature state even though it is not a routinely used material. A niobium based alloy with 1% zirconium added for strengthening has been selected for the outer and inner shells, with niobium mesh being used for the wick and bridge within the heat pipe. It is felt that this alloy presents the best combination of strength, chemical compatibility, and ease of fabrication for the task.

The second important issue was that of design of the heat pipe, both from the standpoint of function, and secondly for fabrication and operational reasons. The isothermal furnace liner has a more complex geometry than the heat transfer application for which the heat pipe is conventionally used. In contrast, this type of heat pipe, or isothermal liner requires that the material being processed be maintained at uniform temperature within a cavity. The evaporator part of the heat pipe is therefore on the outside surface of an annular pipe with the condenser at the inner surface. The wick structure is required to operate in two directions. First it has to attain and maintain the condenser temperature at the same temperature as the evaporator, and secondly it has to maintain that temperature all along the inner surface of the inner part of the tube. Desired heat transfer is therefore in two dimensions with a more complex circuit for the return on the condensed liquid to the evaporator. The wick structure therefore has to bridge the gap from the outer tube to the inner tube wall. From the functional standpoint, in order to facilitate precise alignment of the load within the heat pipe an early design criterion was that this annular tube be open at both ends, allowing one to view the positioning of the load both on insertion and during any translation. Such a geometry puts considerably more strain on the welding of the end caps to the main body. There is an anticipated temperature

II. MSAD Program Tasks — Advanced Technology Development

variation between the inner and outer surfaces of the pipe during heat up before the lithium vapor pressure is actively isothermalizing the assembly and the potential for the end welds to crack is that much higher.

The aim is to produce heat pipes capable of operating within 0.75 °C of the required temperature over long periods of time (a matter of days), and with the ability to withstand many cycles between room and the operating temperature. Following preliminary tests, the heat pipes will be incorporated into a new crystal growth facility at MSFC.

Task Significance:

The instrument presented here will have a considerable impact on materials science. While specifically aimed at manned flight applications, ground-based benefits are equally important. A high temperature heat pipe of the specifications described does not exist for crystal growth and will immediately produce dividends for those growing crystals and doing other materials science in the temperature range 1100 °C - 1500 °C. In flight experiments, where investment per mission is so high, it is essential that thermal conditions for experiments be optimized so that science returns can be maximized. The heat pipe is a major step forward towards reaching this goal.

Progress During FY 1996:

In 1996 suitable test articles have been fabricated and extensive testing has been completed satisfactorily. The final assembly of the first of the three heat pipes is imminent, and the test furnace system, which incorporates both thermocouple and fiber optic measurement capability, is being assembled at MSFC.

This project originated in Fiscal Year 1995 and was planned as a four-year effort to include also the moving gradient heat pipe furnace. After the first year, the emphasis was changed and the effort was exclusively devoted to the fabrication and testing of the high temperature isothermal liner. To complement the development program, dialog has been initiated to establish the protocol for incorporation of the liner as an integral part of a furnace module for the Space Station Furnace Facility. As part of the investigation, a survey has been made of the efficiency of operation of heat pipes in space applications, in particular emphasizing those problems which have occurred in the past. The data base of liquid metal heat pipes operation is no longer zero, due to the flight of the Liquid Metal Thermal Experiment (LMTE), operated by the Phillips Air Force Laboratory in May 1996. Initial results have indicated that the experiment was successful.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/94 EXPIRATION: 10/97

PROJECT IDENTIFICATION: 963-70-07

RESPONSIBLE CENTER: MSFC

II. MSAD Program Tasks — Advanced Technology Development

Space Bioreactor Bioproduct Recovery System

PRINCIPAL INVESTIGATOR: Steve R. Gonda, Ph.D.

NASA Johnson Space Center (JSC)

CO-INVESTIGATORS:

Pellis, N.R.

NASA Johnson Space Center (JSC)

Tsao, Y.-M.

KRUG Life Sciences

Lee, W.

KRUG Life Sciences

Task Objective:

The major milestones for the first year were to complete a survey of current technology for cell culture bioproduct separation and recovery and to begin the development of the BRS test bed. The specified objectives for FY96 were to conduct a survey of and evaluate the existing technology for cell culture product separation and recovery. Based on the evaluation results, bioproduct recovery system components and candidate cell products, as well as cell lines, will be selected. These components will be used to initiate the development of the BRS test beds.

Task Description:

The objectives of the proposed work are to complete the procurement and fabrication of the BRS test bed components and integrate them into a functional system. Major BRS test bed components are the BRS cartridges, affinity chromatography components, membrane filters, bioreactors, and analytical equipment. BRS prototype affinity cartridges will be designed, fabricated, and evaluated against the established operational and science requirements for BRS. Two cell lines/bioproducts have been selected for evaluation in the BRS; a recombinant protein — beta-galactosidase, and an anti-cancer biomolecule from conifer plant cells.

1. Test Bed Development and Operation. Bioreactor systems will be integrated into the test bed to support operational and science requirements. Bioreactor cell culture protocols for each of the selected cell lines will be developed and standardized.

2. Select Candidate Cell Products and Cell Lines. Based on our literature search and evaluation, two biomolecules will be selected as the candidate bioproducts to be recovered and preserved using our BRS. The bioproducts and the corresponded cell lines will be used as model systems to develop the proposed BRS.

Task Significance:

The utilization of microgravity for mammalian cell and tissue culture research and applications is a major focus of NASA's biotechnology program. Over 30 cell lines have been grown in the NASA bioreactors. As one of the major tissue culture applications, space bioreactors will be used to produce high-value added bioproducts and bioactive substances that attend tissue development. At present, an automated, semi-continuous space bioreactor (EDU) is under development at the Johnson Space Center.

There is a growing demand from MSAD funded biotechnology investigators for recovery of cell culture bioproducts during long-duration bioreactor cell culture in the Mir BTS Facility and ISSA BTF. Some of these bioactive macromolecules secreted by mammalian cells exist in low concentration in the bioreactor effluent. Development of purification and enrichment technologies to recover products from dilute aqueous effluent in one of the key needs in today's biotechnology.

The current low temperature stowage facilities available in space vehicles are limited for storage of large volumes of collected bioreactor effluent. Without preservation during the long mission increments, the diluted bioproducts will degrade. Development of long-term bioproduct preservation method(s) and strategies becomes a significant issue.

Progress During FY 1996:

A survey of current technology for BRS components is completed. Procurement of components for the BRS test bed is in progress. designs for BRS cartridges are complete and production of prototype cartridges is in progress. Candidate cell line and bioproducts are under review and two candidates have been identified.

II. MSAD Program Tasks — Advanced Technology Development

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 5/96 EXPIRATION: 5/00

PROJECT IDENTIFICATION: 963-40-23-14

RESPONSIBLE CENTER: JSC

II. MSAD Program Tasks — Advanced Technology Development

Microgravity Combustion Diagnostics

PRINCIPAL INVESTIGATOR: Mr. Paul S. Greenberg

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

Griffin, D.W.

NASA Lewis Research Center (LeRC)

Vander Wal, R.L.

NYMA, Inc.

Weiland, K.J.

NASA Lewis Research Center (LeRC)

Piltch, N.D.

NASA Lewis Research Center (LeRC)

Task Objective:

Currently available diagnostic instrumentation for achieving these objectives has been extremely limited, consisting primarily of conventional film-based imaging systems and intrusive temperature and velocity probes, such as thermocouples and hot wire anemometers. This situation has arisen primarily because of the unique and severe operational constraints which are inherent in the conduct of reduced-gravity experimentation. It is the recognition of this pressing need to provide diagnostic systems of greater sophistication that has motivated the existence of this particular development program.

Task Description:

For a variety of reasons, predominant emphasis has been placed on the development of optical diagnostic techniques. Principal among these is the relative fragility of the physics and chemistry of reduced-gravity systems relative to their 1-g counterparts. The action of buoyancy-induced convection is vigorous when compared with the dominant mechanisms associated with reduced-gravity phenomena, such as surface tension and thermal and concentration driven diffusion processes. The essentially nonperturbative nature of optical measurement techniques is therefore extremely appropriate in this context.

Optical measurement techniques are, in general, well-suited to the acquisition of multidimensional data fields (e.g., two- and three-dimensional imaging). This is an important consideration in the present state of understanding of microgravity science, since a clearer understanding of basic phenomenology, including the verification of fundamental length and time scales and dominating physical mechanisms is still being developed.

Task Significance:

The success in achieving a significant scientific return from existing and proposed microgravity fluid physics and combustion science experiments depends substantially on the availability of diagnostic systems for the collection of the required scientific data.

Progress During FY 1996:

In the area of full-field infrared emission spectroscopy, calibration of the IR sensitive staring array camera has been conducted. This was accomplished through the use of a blackbody radiation source and several infrared bandpass filters. An end-to-end calibration is required in this case because of the varying response of the detector array and the transmission characteristics of the lens and bandpass filters. All of these elements exhibit behavior that is wavelength dependent; the detector response may exhibit nonlinearities with respect to absolute intensity as well. The response of the detector array has been observed to be nearly proportional to blackbody intensity when narrow band filters are employed. As a first step in exploiting this calibration, images of radiating thin filament fibers suspended in jet flames have been obtained. The resulting data will be compared to thermocouple measurements of the hot gases above the flame that were obtained simultaneously.

During this year, a blackbody source needed for camera calibration was recalibrated. This is necessary to characterize the camera response for quantitative measurements. Also, an infrared monochromator with lead salt detector was configured to acquire wavelength resolved emission scans. Future plans include the acquisition of bandpass filtered images, and multi-point temperature measurement using thin-filament pyrometry.

II. MSAD Program Tasks — Advanced Technology Development

A preliminary literature search was made investigating the inverse problem wherein infrared emission measurements are inverted to provide temperatures and concentrations of selected species. The present search focused on references comparing modelling efforts and experimental data for an experimentally tractable (soot-free, relatively simple chemistry, straightforward geometry) combustion system. Published infrared spectra of some laboratory flames, such as a Bunsen-type natural gas flame, have also been found.

In addition, a new Phase I SBIR work entitled "Analysis Tools for Spectrally-Resolved and Broad-band Infrared Imaging Data" was successfully proposed by Aerodyne, Inc., with much of the proposal being based on discussions with ATD personnel regarding the data analysis requirements for both bandpass filtered and spectrally resolved infrared imaging data obtained by several microgravity combustion experiments. The proposed work involves a survey of available optimizer routines, an evaluation of their adaptability to the Aerodyne Radiation Code, and the fitting of synthetic data with and without synthetic noise added in preparation for the fitting of real data.

The Phase I effort was successfully completed, and demonstrated that spatial correlation data in conjunction with state equation relationships can be exploited to obtain accurate reconstructions of both temperature and species concentration fields in selected combustion systems of interest. The Phase II SBIR proposal, however, did not receive approval for funding, predominantly due to the review panel's comments regarding commercial applicability.

Independent of but complementary to this ATD, the Phase II SBIR contract with SSG, Inc. for the development and delivery of an infrared imaging spectrometer capable of supplying spatially and spectrally resolved images made much progress and is nearing its end. All requirements for the instrument have been finalized and the hardware components are complete. The design of the system is such that the system can be accommodated in an aircraft rack for reduced-gravity experimentation and the components have been ruggedized as much as possible. An aircraft rack is under construction. Integration of the hardware and software is being done now, after replacement of the flawed Pentium processor in the computer. The PI was invited to present a talk on the contract results at the Third International Microgravity Combustion Workshop. All hardware and software systems have been delivered to LeRC and are presently undergoing acceptance testing in the laboratory.

Laboratory tests have been conducted on the SSG infrared imaging spectrometer using both spatial resolution targets and spectral emission standards. Results indicate that the instrument is performing as specified. Subsequently, spatially- and spectrally-resolved images of several flames were obtained in the laboratory. The analysis of this data was intended to be completed under a Phase II SBIR with Aerodyne, Inc. Since the Phase II proposal was not selected for funding, other mechanisms for pursuing this analysis are being explored.

Spectrally-resolved images using fixed band-pass filters were obtained from smoldering and combusting solid fuel samples. This effort will ultimately support the science objectives of Drs. Kashiwagi, Altenkirch, and T'ien. Solid surface temperature profiles were reconstructed for regions exterior to the combustion zone where representative values for solid phase emissivities are available. A polynomial interpolation scheme was employed for the internal region and char front. These results will be compared with experimental data obtained in a temperature-controlled oven to test assumptions regarding the emissivities corresponding to these locations.

Efforts supporting two-dimensional species and temperature measurements were initiated with the completion of the procurement process for the titanium:sapphire laser. The laser, built by Continuum, Inc., was installed into a new laboratory room in the Space Experiments Laboratory. Through frequency doubling, tripling, and mixing of the titanium:sapphire fundamental output, light in the blue and ultraviolet has been successfully generated. These lines cover the wavelength regions of 431 nanometers and 308 nanometers, providing the ability to perform laser-induced fluorescence measurements of the CH and OH radicals, respectively. This laser system is currently being characterized as to its operational capabilities. Optics and other support equipment (burners, chamber, etc.) to perform Rayleigh scattering, laser-induced fluorescence, and other optical diagnostics have been obtained and are presently being assembled.

Characterization of this new device began by looking at water, which is optically active throughout the fundamental wavelengths of the laser and allowed familiarization of the laser system without the worry of frequency conversion. A photoacoustic cell and associated electronics were constructed. Excitation of various absorption bands of water at room temperature can be detected, thus serving as a frequency marker to reference the laser tuning process. Synchronization of the laser pulses, data collection systems, and wavelength tuning has also been implemented.

II. MSAD Program Tasks — Advanced Technology Development

Next, the frequency doubling capabilities of the laser were characterized. Several millijoules of light could be produced at 390 nm, which is in the range of one of the CH radical electronic transition. The laser was set up to automatically scan the frequency conversion crystal angle as the wavelength is scanned. The scan rate for auto-tracking was determined to be at least 0.1 nm/sec. The tuning range of the laser when optimized at a particular wavelength is greater than 60 nm, although the auto-tracking alignment must be slightly realigned for good tracking at roughly 20 nm intervals.

A Bunsen-type methane/air flame was set up and a point, laser-induced fluorescence signal of the CH radical present in the inner cone of the flame was obtained with the use of a monochromator and photomultiplier tube detection system. The peaks were assigned using published line positions. From the difference in the actual versus measured wavelength of about 2.32 nm, a wavelength calibration of the laser can be made.

The solid-state laser system was relocated to a new laboratory to minimize conflicts with the extensive soot production from the laser-induced incandescence (LII) ATD which lead to the damage of several optical components. The laser system was characterized at 308 nm, which allows the detection of the OH radical, one of the most important flame front markers. The pulse energy as a function of wavelength or the tuning curve, and the shot-to-shot stability were measured in this wavelength range. The pulse energy and stability are both within specifications and sufficiently good for OH detection experiments. Writing of a computer program for the control of wavelength and multi-channel data acquisition has been completed.

In preparation for imaging laser-induced fluorescence experiments, a demonstration of the synchronization of the pulsed laser, gated image intensifier camera, and digital frame-store capabilities was conducted. The first demonstration was for the fluorescence imaging of an acetone-seed, non-reacting jet. The image was obtained at an excitation wavelength of 266 nm using the new laser for the LII/ATD. The synchronization set-up is identical for a combustng system, but is easier to accomplish for a system with essentially zero background, as there is no flame. The jet had a Reynolds number of roughly 2000 based on the nitrogen flow.

Also completed during the past year was the rework of the optical paths of the pulsed Ti:Al₂O₃ laser systems. This achieves increased stability of the output in the UV, and reduces movement of the probe beam during wavelength scanning. The latter permits excitation scans for temperature measurements. This improved capability has been utilized to acquire data in laboratory flames. Simultaneous absorption data was also obtained, and the combination is being analyzed to provide both temperature and absolute OH number density. The prior demonstration of the synchronization of the laser, imaging array, and computer digitizer permits the extension to both line and imaging configurations. Multi-wavelength Rayleigh scattering experiments are presently being configured using parasitic optics to permit the parallel completion with LIF experiments. In similar fashion, initial experiments will focus on point measurements, followed by the extension to multi-dimensional measurements.

Also in support of the laser-induced fluorescence experiments, several OH and CH chemiluminescence images were obtained for burning methanol and decane fiber-supported droplets. These experiments were performed at low pressure in an attempt to simulate low-gravity conditions and obtain an approximate signal level of the OH and CH chemiluminescence intensity to guide potential reduced-gravity measurements of the same. The methanol images reveal significant emission from OH A-state and CH A-state electronically excited radicals. The CH emission may be used as an alternative to the OH emission in determining the position of the flame front. Since emission is seen from CH A-state radicals, this hints that other reactions may produced CH in the C-state, whose emission overlaps that from the OH radical. Detailed high resolution spectroscopic measurements are needed to discern the relative contribution of the CH emission to the light collected near 308 nm. Previous modelling by Prof. Dryer does not predict the formation of CH in the combustion of methanol droplets. These observations provide an alternative method of spectroscopically determining the flame front position during the burning droplet lifetime, provide input for the theoretical modelling of the combustion chemical mechanism for methanol droplets, and provide a caution against the assumption that light emission centered at 308 nm is due solely to OH radical emission. The decane droplet chemiluminescence images provide a point of comparison for the methanol droplet.

During this period of performance, a related effort was undertaken to determine oxygen spatial extent and concentrations profiles in flames, using non-intrusive optical techniques. Absorption in the ultraviolet Schumann-Runge bands was selected based on sensitivity, compactness of the apparatus, and ability to measure hot oxygen without interference from ambient oxygen. In addition, the same technique would similarly be able to

II. MSAD Program Tasks — Advanced Technology Development

measure ambient oxygen by suitable choice of wavelength.

The absorption spectra for these bands were modeled with a simulation program obtained from Princeton University, over a temperature range from ambient to 2000 K. Several groups of transitions were identified that promised high sensitivity and minimum interference by ambient oxygen. Since several excited vibrational levels are populated and can be probed in this region, temperature can be determined from these measurements. The simulated spectra at 300 K and 1500 K show spectral regions, such as that near 195 nm, where hot oxygen absorbs but room temperature oxygen does not.

Also considered are the Franck-Condon factors as a function of wavelength and vibrational quantum number. The Franck-Condon factor is the vibrational contribution to total transition probability. Calculated values for transition probabilities shows that there is a four order of magnitude increase from $v'' = 0$ to $v'' = 4$. The product of Franck-Condon factor and population of that state is nearly constant within a factor of ten for states from $v'' = 0$ to $v'' = 4$ at flame temperatures. Therefore vibrationally excited states can be detected at nearly the same sensitivity as $v'' = 0$, while also allowing temperature determination from the spectra. The vibrationally excited states have the additional advantage of being shifted toward longer wavelengths where transmission through optical elements will be improved.

Measurements are planned in line-of-sight absorption, point fluorescence, and planar imaging. A lightweight, compact, low power xenon arc lamp has been purchased with a repetition rate of 300 Hz and sufficient intensity in the sub-200 nm region for these measurements. UV optics (lenses, filters, and a monochromator grating) have also been obtained. Initial absorption measurements are in progress.

Exciplex thermometry experiments are being performed utilizing a small pulsed nitrogen laser operating at 337 nanometers. The objective is to utilize this method to measure the temperature of a vaporizing droplet, and extend the technique to a burning droplet. Exciplex thermometry utilizes the ratio of fluorescent intensities of an excited state monomer and exciplex compound (formed through the interaction of an excited state monomer and ground state partner). By referencing this ratio of fluorescence intensities to calibration measurements in which the intensity ratio is measured at known temperatures, the temperature can thus be determined. This technique has been applied to measure the volume average temperature of a fiber suspended droplet in an inert atmosphere in response to heating by a hot wire coil surrounding the droplet. The system in this case is hexadecane doped with PYPYP. Application of exciplex thermometry to burning droplets remains a challenge as the fluorescence from the monomer and exciplex are quenched at different rates in the presence of oxygen. Current efforts are aimed at addressing this issue.

Several hardware modifications were accomplished to enable these investigations. These include: a) a refurbishment of the existing droplet combustion chamber to serve as a glove-box for performing experiments in an oxygen-free environment, b) the design and fabrication of a glass vacuum system for degassing solutions of dissolved oxygen, (the capabilities of this system have since been adopted for use by the Droplet Combustion Experiment (DCE) program) c) the design and fabrication of a new calibration cell, d) dual fluorescence detectors for measuring the fluorescence of the monomer and exciplex compounds simultaneously, independent of the experimental geometry, e) an improved hot-wire ignition mechanism, and f) the identification and procurement of new potential exciplex compounds based on a survey of the open literature.

Several new exciplex compounds and fuel combinations were tested for their temperature dependence and fluorescence signal levels. The two most promising systems were identified as PYDMP/Decane and PYPYP/Decane. The PYDMP, a new intramolecular compound, was previously unavailable and neither exciplex compound had been tested in combination with the fuel decane.

Most significantly, these compounds are intramolecular compounds which form an exciplex compound through an intramolecular rearrangement. Since the two 'parts' of the molecule are in relatively close proximity to each other, far lower concentrations can be used. It has been routinely observed that intermolecular compounds require significantly higher concentrations for an exciplex compound to form. The resulting drawback is that with such high concentrations, not only is the burning rate constant of the droplet altered (a significant perturbation), but the droplet is frequently difficult, if not impossible to ignite. Furthermore, the differences in vapor pressure between the fuel and dopant dictate that the relative concentration of the dopant varies throughout the burning process.

II. MSAD Program Tasks — Advanced Technology Development

The overall lower concentrations required by the use of intramolecular compounds tends to reduce this undesirable effect.

The fluorescence of an exciplex compound and monomer is also sensitive to the presence of oxygen. While adequate signal levels are attainable in the presence of oxygen, its quenching effect on the fluorescence differs for both the monomer and exciplex compound. Calibration experiments are performed steady-state, where in order to bring the solution temperature to a predetermined level, a period of several minutes is required. In contrast, the ignition of a fuel droplet occurs within a few seconds. As the temperature of the droplet varies both temporally and spatially (which is what is desirable to measure experimentally) during the ignition and burning stages, the oxygen concentration in the solution will vary as well, owing to the temperature dependence of the dissolved oxygen concentration. Since the fluorescence intensity of exciplex to monomer is a strong function of both temperature and oxygen concentration, the inferred temperatures based on fluorescence intensity ratios will not necessarily accurately reflect the true temperature of the droplet.

It does not appear feasible to begin with an oxygen free fuel droplet (for a single fiber-supported droplet) and accomplish ignition in air before significant changes in the fluorescence intensities occur due to oxygen dissolving in the solution. Given the rate of diffusion of oxygen to the droplet, it is observed that the dissolving of oxygen into the solution occurs almost instantaneously.

The temporal and spatial variation in the oxygen concentration essentially renders a suitable calibration procedure exceedingly difficult, if not impossible. Thus our approach involves a comparison of droplet temperatures prior to ignition for an oxygen-free fiber-supported decane droplet (doped with either of the two indicated exciplex forming compounds) residing in an oxygen free environment, and an identical aerated decane droplet residing in air. The calibration for each experiment will be performed in the appropriate oxygen-free or air environments. Comparison of the temperatures of the decane droplet during the ignition process for both sets of experimental conditions (with calculated temperatures being based on the appropriate calibration experiment) will be made for both experiments to empirically determine how much error may be incurred in an actual experiment performed in air referenced to a calibration procedure performed under similar conditions. If similar temperatures are indicated, then the technique should also be applicable to burning droplets. At a minimum, the technique is clearly applicable to studying droplet temperature prior to ignition, a situation of expressed concern to several MSAD funded investigators.

During the course of these experiments the nitrogen laser failed, preventing a direct comparison of the two sets of experimental conditions. It was possible, however, to perform the calibration experiments in air. Using the resulting functional fit describing the calibration curve, the experimentally determined fluorescence intensity ratio of a fiber-supported oxygen-free decane droplet in an oxygen-free environment was used as an input. The ignition point is based on the observed time to ignition for an identical droplet in an air environment. Rough measurements have indicated that the very low concentrations of these intramolecular exciplex compounds do not change the burning characteristics of the host fuel. Additionally, the ratio of thermal conductivity of air to pure nitrogen is nearly unity, thus validating the determination of the ignition point in the oxygen-free environment based on measurements performed in air. Most importantly, the inferred radially averaged droplet temperature is significantly lower (~ 90 Celsius) at the point of ignition than the boiling point of decane (~ 175 Celsius). Preliminary results from the PYDMAP exciplex compound in decane yield similar results. Thus our initial conclusion indicates that hot-wire ignition does not bring the bulk droplet temperature near the fuel boiling point. The accuracy of these results however, requires a comparison to the oxygen-free experiments as previously discussed.

In the past year, a new flowing exciplex calibration cell was designed and constructed. This cell prevents degradation of the exciplex test solution during the heating process by minimizing the preparation and exposure time under elevated temperature conditions. This cell was also fitted with a custom-made dual wavelength fiber-optic detection system. This provision allows for simultaneous detection of monomer and exciplex emissions, and eliminates problems with selective detection due to spatial positioning errors. Two new intramolecular compounds (PYDMAP and PYPYP) were procured and characterized. A useful result is the demonstration of the PYDMAP/decane exciplex system that extends the useful temperature range up to the boiling point of decane. Experiments were then performed to assess the relationship between oxygen quenching and a priori calibration in oxygen free conditions. The observed differences in absolute temperature were significant (maximum deviation of 30° C), although it is conceivable that repeatable calibration constants can be obtained for specific fuels and geometries, since reasonable detection sensitivities were demonstrated. Nonetheless, the utility as a diagnostic

II. MSAD Program Tasks — Advanced Technology Development

for transient thermometry in oxygen free surroundings has been demonstrated.

Point-wise and imaging velocity measurements are also in progress. Addressing the former, compact, solid -state laser doppler velocimeter modules have been obtained on loan to supplement the module being completed under contract. This module is implemented for coaxial backscatter measurements, utilizing common optics for simultaneous transmission and detection. This simplifies the experimental geometry, and eliminates the requirement for precise alignment of separate transmission and collection sample volumes. Acceptance tests of the optics module were performed during September of 1993 at EG&G's facility in Montreal. The results of these tests indicate that the unit performed as per specification. A comparative basis for the resulting performance was afforded by the availability of a pair of similar units presently in use in our laboratory. These units were loaned from the David Taylor Institute of the Naval Research Laboratory. Both the EG&G and NRL units employ diode laser sources operating at 780 nanometers, delivering approximately 15 milliwatts at the sample volume. Both units also employ DC coupled, avalanche photodiodes (APD) operating in the sub-geiger module (i.e. analog detection as opposed to photon counting). For comparable optical power present at the sample volume, the EG&G module affords an improved detection sensitivity by roughly a factor of four. A two-fold improvement is evident directly from the indicated data, whereas the additional factor of two results from F# considerations; both modules employ a collection aperture of 50 millimeters, but the EG&G module has a working distance which is 1.4 times as long. Also visible in the data is the considerable improvement in the spatial definition afforded by the EG&G module. The radial profile of the sample volume is very close to the predicted value of 100 microns, and much more closely resembles the $1/e^2$ profile associated with the source. The NRL unit, in contrast, has inferior beam shaping optics, resulting in a series of unwanted "wings" which contribute to the overall scattered signal.

Upon receipt of the EG&G optics module at LeRC these tests were repeated. Unfortunately, two anomalies in the performance of the system were observed which were not seen previously. The first corresponds to a misalignment between the transmitted and detected sample volumes. Data was collected to indicate the output of the avalanche photodiode detector as a partially reflective target was translated along the optical axis. It is seen from the resulting plot that the detection sensitivity peaks approximately 20 millimeters behind the sample volume as defined by the transmitter. Because the detection optics operate at a conjugate ratio on the order of 10:1, this is indicative of a misalignment of the detector by roughly two millimeters. This distance was later revealed to correspond to a shift in the distance between the entrance window and sensor surface that had been altered in the final version of the detector. This change had evidently not been indicated in the final configuration drawings, and hence had become inadvertently misaligned in the final cleaning, purging, and sealing of the module which occurred prior to shipment. The second anomaly relates to 50 KHz bleed-through from the detector high voltage power supply, and was traced to a leaky by-pass capacitor. The module has subsequently been returned to EG&G, where these problems were addressed.

When the module was received from EG&G, these same tests were revisited. The results were favorable, indicating that the identified problems had been adequately rectified. A number of additional tests were then conducted, serving to both validate the module's performance, and as a basis for further comparison with the existing NRL units. The actively cooled APD utilized by EG&G affords a net increase in detection sensitivity of eight fold. A similar increase in signal to noise ratio (SNR) is not achieved, however, due to the larger noise floor attributable to the initial design goal of incorporating the high voltage generation circuitry internal to the module. Factoring in this consideration provides an improvement in SNR of roughly 3:1. This improvement affords the use of smaller seed particles, and offers the possibility of confocal masking to improve the axial spatial resolution. Also evident is an improvement in sample volume geometry. The anamorphic prisms effectively circularize the output, providing a $1/e^2$ diameter that corresponds well with the design specification of 150 microns. This is not to say, however, that true diffraction limited performance has been achieved. A circular stop preceding the beam splitter does result in some observable diffraction at the sample volume; this is manifest by the occurrence of modulation fringes external to the nominal $1/e^2$ envelope. Scattered signals resulting from particles traversing these regions are normally rejected by frequency domain filtering. The modulation in regions external to the sample volume resulting from residual diffraction effects reduces the effectiveness of this filtering process. The increase in detection sensitivity, however, affords the possibility of enhanced axial rejection through confocal masking. Because confocal masking is achieved through the use of a central obscuration, a loss in effective collection efficiency results.

The difference in detection sensitivity also influences the minimum resolvable scattering cross section (i.e. particle diameter for a specified seed material) that is required. Velocity field data from a droplet seeded jet was obtained from

II. MSAD Program Tasks — Advanced Technology Development

distribution, particularly in the range of 0.5 micron and below, and thus provides a useful demonstration of this specific point. In the more laminar core flow, the impact of the droplet size distribution is diminished regarding the ability to accurately follow the flow. At larger radii, the ability to track increasing levels of turbulence intensity becomes biased towards smaller droplet diameters. The relative decrease in detection sensitivity afforded by the non-cooled APD begins to underpredict the level of turbulence intensity, and biases the estimate of the mean towards lower velocities. This is also reflected in the corresponding data rates, wherein the more sensitive APD is seen to more adequately resolve a larger percentage of the net droplet flux. The more sensitive detector provides velocity estimates over a broader range of SNR, produces higher overall data rates, and a broader velocity probability density function.

Also acquired during this period of performance is a novel LDV signal processor. This processor belongs to a relatively new generation referred to as burst-resolved, and implements the calculation of complete frequency spectra at a maximum rate of ten thousand spectra per second. This particular device possesses several advantageous features useful for the conduct of reduced gravity experiments, most notably its configuration as a pair of stand-alone circuit cards which plug into the bus of a conventional PC. Also of significance is the ability to operate as a digital transient recorder. This option is useful for performing experiments of limited duration, such as in the drop towers or reduced gravity aircraft. The complete set of raw data can be rapidly digitized and archived, allowing post processing and velocity estimation to be performed off-line. Another attraction is the interactive graphical user interface, which enhances the ability of the user to perform real-time assessments of the attributes of the incoming signals, and implement parameter settings to optimize the accuracy of the resulting velocity estimates. This latter feature is viewed as particularly favorable under the scenario where measurements are to be performed by an operator of somewhat lesser experience and expertise, such as a crew member.

This processor also includes provisions for synchronization and control of external events. The principal motivation for this capability is to provide an integrated system for performing rapid spatial scans. To accomplish this function, the output beams are steered by a pair of galvanically controlled turning mirrors. Because of the coaxial optical configuration, the sample volumes corresponding to the transmitting and receiving optics coincide. A compact, high bandwidth scanning head with compensating electronics to provide constant linear scan velocity has been identified, and includes provisions to interface with the processor's synchronization and control protocol.

This device is now being driven via control waveforms directly synthesized by the computer system contained in the 2.2 second drop package. The computer simultaneously generates synchronization flags for use by the LDV signal processor. This scanning capability has been verified in the laboratory to achieve the desired scan rates and positional accuracy, and is presently being integrated into the 2.2 second package.

In the area of Particle Image Velocimetry, a specially configured, pulsed Nd:YAG laser was received. This laser was designed to emit a 4 pulse burst every second; shots in the burst are repeated at a rate of 1KHz. It also can produce single pulses with a 30Hz repetition rate, although the energy produced is much less. The output is frequency doubled to 532 nanometers via an internal doubling crystal. This laser uses a recently developed folded-resonator configuration, resulting in an extremely compact optics package. Although some "tweaking" of this system was required by the manufacturer, subsequent acceptance testing of this unit has validated that the specified performance has indeed been achieved. In addition to the rugged, compact packaging of the optical head, this laser system is configured so as to be compatible with operation in either the NASA Learjet or KC-135 aircraft.

Following receipt of the laser, a cyclonic insertion fluidized bed seed chamber was designed and fabricated. This seeder is intended for use with gas jets which are identical to those in use by investigators currently funded under the MSAD program. Clear acrylic was used as the material so that the flow structure in the interior could be viewed. Testing revealed that the injection velocities were too low to entrain sufficient numbers of particles due to the diameter of the inlet port and the relatively small mass flow rates employed in these experiments. Additionally, the flow tended to "tunnel" through the particle bed which further precluded entrainment. Based on these results, a new design was developed, with the goal of developing fully-turbulent flow inside the seeder plenum. The diameter of the burner, which forms the outlet of the chamber is 1.65 mm. With an inlet diameter of approximately 0.1 mm, a Reynolds number of roughly 2000 inside the seeder was achieved. This design was tested using a new type of seed particle known as "Microspherical Feathers," manufactured by Osaka Gas and discovered by Paul Greenberg while working on the LDV portion of this project previously described. These particles are essentially hollow spheres of silicon dioxide, and are extremely monodisperse. They possess extremely large scattering cross sections and small

II. MSAD Program Tasks — Advanced Technology Development

effective hydrodynamic diameters, both properties being advantageous for this application. Initial testing showed that the particle entrainment was excellent and velocity vectors were determined using images captured both live and from a pre-recorded sequence recorded in Sony BetaCam format. To simplify the experimental configuration, the illumination for these tests was provided by a CW argon-ion laser. The data reduction algorithm being utilized was developed by Dr. M. P. Wernet of the Instrumentation and Control Technology Division of LeRC, and has been previously described.

In order to measure velocity maps, the video system and laser must be properly synchronized to insure that an image is recorded on all frames. Additionally, particle images must appear as points and not streaks so that the software can accurately locate the centroid of each particle image. During this last reporting period, the synchronization of the pulsed Nd:YAG laser and video was successfully demonstrated, resulting in the capability for flow analysis in a range between 5 and 150 cm/sec. Given that the sub-buoyant velocity range is 5-40 cm/sec, the current setup can easily accommodate most phenomena of interest. Velocity maps were recorded with the limitation on measurement accuracy being determined by the resolution of the array currently being used.

Previous analysis of particle images was performed using software that was written using support from the previous ATD award. However, that software required 5 images to accurately determine velocity vectors. As a result, flows with curvilinear characteristics were difficult to accurately quantify. More recent versions of the software have incorporated fuzzy logic algorithms, which reduce the image requirement to only two. This software has been used with data generated from the Droplet Combustion Experiment (DCE) in the 5.2 Second Tower to compute velocity vectors for the large soot aggregates generated during the burn. Due to the illumination system used, these numbers were two-dimensional projections of a three-dimensional velocity. Based on the results to date, Microgravity Combustion Diagnostics (MCD) personnel are assessing designs for an improved illumination system to better record the flow.

As PIV technology is transferred to investigators external to the MCD group, investigators frequently want to know the appropriate design parameters required to properly engineer a PIV system. To develop an intelligent design, the intensity of the scattered light and sensitivity of the array must be known. While the latter is provided by the manufacturer, the former must be computed from light scattering theory. To that end, software was acquired to calculate intensity factors for Mie scattering. These results are used directly to determine intensity distributions at the receiving optics, or integrated using MCD-developed software to determine the scattering cross section. Use of these two codes allows direct engineering of PIV systems in terms of required source strengths, scattering cross sections, integration times, and fields of view. The capability has since been made available to the general research community. Also derived and disseminated is a program that describes the propagation of Gaussian beams and allows the design of optical systems to generate points, lines and sheets of arbitrary dimensions using a variety of laser sources.

While the laboratory development is still in progress, the transition to reduced gravity platforms has begun. The initial effort involves a collaboration with Fletcher Miller, technical analyst/monitor for NRA awardee, Fokion Egolfopolous of the University of Southern California. MCD personnel have designed and tested a particle seeder that will be used in the 2.2 Second Drop Tower tests. This seeder is a scaled-up version of the seeder that MCD personnel have been using in the laboratory over the past year.

In addition to assisting Professor Egolfopolous, MCD personnel have taken steps to provide PIV capability in the small drop tower and on the DC-9 aircraft. In the former facility, PIV and LIF would be facilitated by using a large diameter optical fiber to transmit 10-20 nanosecond laser pulses with energies on the order of tens of millijoules. Typical fibers suffer laser damage at those levels, but initial testing with a new fiber type revealed a transmission capability of 15 millijoules at 532 nm.

Suitable focusing optics to couple to the fiber have been integrated with the laser head, and installed at the 2.2 Second Drop Tower facility. This system has now been successfully utilized to acquire particle image field data in reduced gravity. The resulting data is presently under evaluation.

Finally, fabrication was begun on an experiment frame to accommodate the use of the compact Nd:YAG laser on reduced gravity aircraft. This frame will be used as a platform for the laser and will be used in conjunction with a rig from the 2.2 Second Drop Tower to demonstrate gas phase PIV in reduced gravity. We anticipate completing

II. MSAD Program Tasks — Advanced Technology Development

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/92 EXPIRATION: 9/96

PROJECT IDENTIFICATION: 93-2

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Greenberg, P. S., and Ku, J. C., Soot volume fraction imaging. Applied Optics, (1996).

NASA Tech Briefs

Greenberg, P., NASA tech brief: pulsed laser shot counter. NASA Tech Brief, (1996).

Proceedings

Proceedings: Moir, C.I., Greenberg, P.S., and MacGregor, A., "Compact laser velocimeter module." OSA Meeting on Photon Correlation, Capri, Italy, August, 1996.

Presentations

Greenberg, P. and Ku, J. "Soot volume fraction imaging." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28 - August 1, 1996.

Greenberg, P.S., "Challenges and Capabilities of Microgravity Combustion Diagnostics." The Third International Workshop on Short-Term Experiments Under Strongly Reduced Gravity Conditions, Bremen, Germany, July, 1996.

High Resolution Pressure Transducer and Controller

PRINCIPAL INVESTIGATOR: Dr. Ulf E. Israelsson

Jet Propulsion Laboratory (JPL)

CO-INVESTIGATORS:

Michelson, P.

Stanford University

Lipa, J.

Stanford University

Barmatz, M.

Jet Propulsion Laboratory (JPL)

Task Objective:

The objective of this project is to develop high resolution pressure transducers and controllers with many orders of magnitude better performance than those presently available commercially. The main use of these devices will be for fundamental science investigations in the area of low temperature physics at helium temperatures.

Task Description:

Two types of pressure transducers will be developed for use in the 1 to 10 bar pressure range. The first will utilize a capacitive readout technique and will be capable of operating at any temperature from 300K to 2K. The second will utilize inductive readout by means of a SQUID and will operate at helium temperatures only (2K to 7K). The expected resolution of these transducers are about one part in 10^{10} , and they will dissipate negligible amounts of heat when operated. The pressure controller will be based on similar techniques as the transducers and will be capable of controlling pressures in the 1 to 10 bars range over a limited pressure swing to near one part in 10^{10} .

Task Significance:

The current capability of the MSAD program in fundamental low temperature physics is limited to controlling and reading out one experimental variable, temperature, to sub-nanokelvin resolution at helium temperatures. By providing a similar capability for a second variable, pressure, many new important flight investigations can be performed. An example would be to test the validity of the Universality hypothesis in the theory of second-order phase transitions by performing high resolution measurements of some experimental quantity at several fixed pressures.

Progress During FY 1996:

A prototype capacitive pressure transducer operating in the 2.5 PSI range was constructed using silicon micromachining techniques. It employs a flexible silicon membrane which is sealed to a helium sample chamber with an indium seal. Attached to the back side of the membrane is a thin film capacitor plate. A second thin film capacitor plate is located a short distance away on a fixed block of silicon. Pressure variations in the sample cell will flex the membrane thereby adjusting the relative capacitance of the circuit. The transducer was tested on an existing high resolution thermal platform at JPL. The resolution was determined by making use of the known temperature dependence of the saturated vapor pressure of helium and by applying known temperature changes measured with a high resolution thermometer. With a room temperature reference capacitor, a resolution of better than one part in 10^7 was obtained, thereby demonstrating the viability of the concept. The pressure stability of the transducer was found to be less than desirable. It is believed that this is due to relaxation problems associated with the Indium seal. A new transducer for operation at the desired higher pressures of 1 to 10 bars has been fabricated. Because of its higher operating pressure, the new device will be less sensitive to relaxation problems associated with the indium seal. If need be, harder metal seals can also be used in the current design to reduce the drift to acceptable levels. In order to improve the resolution of the device further, a cold reference capacitor has been fitted to the apparatus.

A prototype inductive pressure transducer has also been constructed. It employs a niobium diaphragm and a superconducting coil in close proximity. The diaphragm serves as a ground plane for the coil. A pressure change will bend the diaphragm thereby changing the inductance of the coil. The inductance change is detected with a DC SQUID sensor at low temperature. The initial test results are very encouraging. At low pressures, a SQUID-limited resolution of about 0.1 billionth of an atmosphere has been demonstrated. The actual resolution is about 1.5 times worse, probably limited by vibration noise. If the measured performance holds up at high

pressures, it is likely that the goal performance on resolution of about 0.01 parts per billion at 10 bars can be achieved.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 1
MS Students: 0
PhD Students: 0

TASK INITIATION: 10/93 **EXPIRATION:** 9/96

PROJECT IDENTIFICATION: 963-01-04-00

RESPONSIBLE CENTER: JPL

Surface Fluctuation Spectrometers for the Characterization of Fluid and Crystal Surfaces

PRINCIPAL INVESTIGATOR: Mr. William V. Meyer

Ohio Aerospace Institute

CO-INVESTIGATORS:

Mann, J.A.
Tin, P.
Rogers, R.B.

Case Western Reserve University
Case Western Reserve University
NASA Lewis Research Center (LeRC)

Task Objective:

We are developing the next generation of easy-to-use surface light scattering technology which compacts an entire optical train and a more sophisticated version of our surface vibration compensation optics into a small fiber optic device. This evolves a non-contact instrument which examines laser light scattered from fluid/fluid interfaces to measure surface tension, viscosity, and (for a well characterized surface) the true surface temperature. The fluid/fluid interface can be either liquid/liquid or liquid/vapor, and it may include a monolayer. The new technique being developed should counteract detrimental sloshing effects (which otherwise make the measurement difficult or impossible) on reflecting interfaces, on transparent interfaces, and those which are neither (which is new).

In this Advanced Technology Development (ATD) project, we are also extending our work in laser interferometry into the area of crystal growth rate measurements. This work parallels the fiber optics portion of the task described above. The fiber optic heterodyning techniques which we pioneered in our former (FY92-95) surface light scattering ATD project are being extended to study interface growth rates in the direction perpendicular to the substrate on which the growth occurs. This technique is ideally suited to study the extremely slow interface velocities encountered during protein crystal growth and when using multiple colors and a unique detection scheme we are developing, it holds the promise of offering absolute displacement measurements over a sub-nanometer to meter range.

Task Description:

While individual surface light scattering (SLS) instruments have been built and used successfully by experienced researchers in isolated labs around the world, the method has been unavailable to non-specialists wishing to use it in their applications. To bring surface light scattering instrumentation out of the lab and into the worlds of space research, the natural environment and the commercial sector, we had to address the problems of vibration sensitivity, size, and optical alignment. We have greatly reduced the size and simplified the optical alignment by developing a fiber optics version of the instrument. We previously addressed sloshing interface concerns with a development which works on transparent and reflective interfaces (our "Cat's eye" optics). We are replacing this technique with one which should work on any interface which allows optical access. With these improvements, surface light scattering instruments are ready to graduate from the research lab and enter the world of applications. Brookhaven Instruments Corporation (among others) has already expressed an interest in making this happen, and designed and provided us with a custom version of an analogue input digital correlator (for our prototyping work). They are now getting ready to put their correlators onto ASIIC chips with the features we need for microgravity research for which both laser light scattering and surface light scattering are being included in the design.

We are continuing to test our improved instrument designs to ensure how accurately they can measure the surface properties of water, ethanol, acetone, silicone oils, and liquid gallium in the presence of ambient laboratory vibration. We are collaborating with a group that has demonstrated that they are capable of making atomically clean gallium, which will allow us to make the first definitive measurements on this system. We are also working with the designers of the Critical Point Facility (CPF) and Alice. They are interested in the possibility of using our surface light scattering techniques in these facilities. We now have a working prototype which combines a working CPF milli to microKelvin temperature control cell (depending upon how we use it) with our surface light scattering instrumentation. The combined instruments are giving us some very nice data. Additional software and interface pinning work is planned to ensure the instruments can work well in a microgravity environment.

II. MSAD Program Tasks — Advanced Technology Development

The protein crystal interferometry work looks at the growth rate of protein crystal interfaces. This should significantly impact not only our understanding of how protein crystals grow, but it will allow us to better control the quality of the crystals which are being grown. The main intention here is to quantify a qualitative art. With this comes better science (control and prediction) and provides a better yield and the best possible quality for crystals grown in space and in the laboratory.

Task Significance:

Surface tension is an elusive phenomena which controls many everyday processes. It is the two dimensional analog of pressure, and it attempts to maintain the smallest possible surface area. It affects cooking, cosmetics (improved formulation), tertiary oil recovery (20-30% more oil can be pumped from the ground), detergents (better wetting of fibers), controlled release and targeted drug delivery, and materials processing such as steel making. Accurate surface tension data is vital in the development of lead-free solders. The multi-billion dollar solder industry is actively searching for lead-free solders because lead leaches from discarded soldered pieces in landfills and contaminates water supplies.

In addition to surface tension data, surface light scattering instruments provide viscosity and, for pure substances, temperature information. Viscosity is the internal friction of fluid (how sticky it is). This affects liquid crystal displays such as the flat screens used in computers and other applications. Surface temperature is useful because it indicates heat transfer rates and the presence of buoyancy driven flow.

The study of surface tension driven phenomena is often masked by gravitational forces which are not present in the reduced gravity environment of a space station or space shuttle. Because of this, a number of space experiments have been proposed and flown which examine the effects of surface tension in near-weightless conditions. Despite their stated interest in surface tension, these experiments have lacked a means to measure it. The surface light scattering instrument described there is a unique and valuable addition to space science in that it permits accurate, non-invasive, in-situ measurements of surface tension and viscosity. From these, one can extrapolate the local surface temperature of a known, clean sample. It has also been developed to be rugged, power efficient, miniature, and flexible in set-up. The knowledge gained with its application will have diverse impacts in many fields of endeavor.

Our work springboards from traditional designs which are bulky and difficult to use because of their extreme sensitivity to vibration. Not only will this new technique much less sensitive to surface slosh (tilt), it can adjust for changes in surface height and will be usable on surfaces which are neither completely transparent or reflective (an improvement on our present anti-slosh optics). For these reasons, surface light scattering instruments, which have never been commercially available should find widespread applications; commercialization is the next logical step.

Growth rate and displacement measurement is valuable for both scientific progress and for industrial applications. The ability to make absolute displacement measurements over a wide measurement range is of extreme interest to many industries (machining, optics, etc.).

Progress During FY 1996:

We have designed and built a new kind of anti-slosh surface light scattering instrument which works on all types of materials. Initial tests, using cells installed in a modified critical point facility show this new design to be very easy to use and able to accommodate a wide range of materials. When the same optical train was used with fluids contained in a conventional flat dish the data degraded considerably (low frequency noise was present because the surface sloshed with several degrees of freedom).

We are designing a multiple wavelength interferometer which should allow absolute displacement measurements. Adding to this a very high resolution (better than 6 Angstrom) extension of quadrature phase detection schemes should allow us to make absolute displacement measurements. We are studying the idea of transforming this interferometer into a surface light scattering instrument by adding an optical mask our new anti-slosh container (which maps all the sloshing effects into one angular degree of freedom which can be compensated for with a simple optics). This has the advantage of being applicable to both high amplitude turbulence and chaos studies and low amplitude protein crystal growth rate and surface tension and viscosity measurements with a single compact fiber optic system.

II. MSAD Program Tasks — Advanced Technology Development

A multiple fiber array system for surface light scattering cross-correlation work has been designed and is nearly completed. It awaits testing.

The first phase of the software needed for such an interferometer (single color with FFT analysis routines) has now been written and tested. It is of sufficient quality that it is being used by a commercial interferometry company.

Continuing work with protein crystal vapor diffusion cell which was built to support L. DeLucas and Bill Wilson. Additional work in this area looks very promising and all parties involved are very interested in continued collaboration.

STUDENTS FUNDED UNDER RESEARCH:				TASK INITIATION:	10/95	EXPIRATION:	9/96
BS Students:	2	BS Degrees:	0	PROJECT IDENTIFICATION:	92-4		
MS Students:	0	MS Degrees:	1	NASA CONTRACT NO.:	NCC3-419		
PhD Students:	2	PhD Degrees:	1	RESPONSIBLE CENTER:	LeRC		

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Presentations

Cheung, H.M., Meyer, W.V., Taylor, T.W., Tin, P., Barmatz, M.B., Biswas, A., Mann, J.A., Jr. "Hardware and software modifications of a commercial laser vibrometer for investigation of high amplitude surface fluctuations with optical tracking." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.

Lant, C.T., Smart, A.E., Cannell, D.S., Meyer, W.V., Doherty, M.P., "The physics of hard spheres experiment - a general purpose light scattering experiment." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.

Mann, J.A., Jr., Farukhi, Z.H., "Surface laser light scattering: data processing and foundations." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.

Meyer, W.V., Lock, J.A., Cannell, D.S., Taylor, T.W., Tin, P., Smart, A.E., Zhu, J.X., Cheung, H.M., Mann, J.A., Jr., "A single wavelength cross-correlation technique which suppresses multiple scattering." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.

Rogers, R.B., Meyer, W.V., Zhu, J.X., Turner, W., Chaikin, P.M., Russel, W.B., "A compact laser light scattering instrument for microgravity research." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.

Taylor, T.W., Meyer, W.V., Tin, P., Mann, J.A., Jr., Cheung, H.M., Rogers, R.B., Lading, L., "A new surface light scattering instrument with auto-tracking optics." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.

Tin, P., Meyer, W.V., Rogers, R.B., Mann, J.A., Jr., Cheung, H.M., Taylor, T.W., "Fiber-Optics surface light scattering spectrometer (FOSLSS)." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.

Tseng, C.S., Meyer, W.V., Tin, P., de Mul, M., Lando, J.B., Mann, J.A., Jr., "Laser light scattering spectroscopy combined with Brewster Angle Microscopy: nCB and polymer monolayers." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.

Zhu, J.X., Chaikin, P.M., Li, M., Russel, W.B., Meyer, W.V., Rogers, W.V., "The structure and dynamics of hard sphere colloidal crystals under micro-gravity with quasi-elastic light scattering." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.

II. MSAD Program Tasks — Advanced Technology Development

The Laser Feedback Interferometer: A New, Robust, and Versatile Tool for Measurements of Fluid Physics Phenomena

PRINCIPAL INVESTIGATOR: Dr. Ben Ovryn

Nyma, Inc.

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this Advanced Technology Development project (ATD) is the evaluation, adaptation and delivery of a novel form of interferometry, based upon laser-feedback techniques, which will provide a robust and versatile, state-of-the-art diagnostic instrument applicable to the measurement of a wide variety of microgravity and ground-based fluid physics and transport phenomena.

Task Description:

Laser feedback interferometry (LFI) differs from conventional interferometry by using the laser as both a light source and as a phase detector. Either a cavity or a semiconductor (diode) laser can be used. LFI can be used either in direct reflection or the interrogating beam can pass through the sample and then be reflected into the laser.

The instrument being developed under this ATD is a robust, phase-measuring device (with simultaneous imaging of the sample) which can determine both slowly time varying and dynamic phenomena over a microscopic and macroscopic field-of-view. Since the interferometer can be used to count fringes, there is no upper limit to the size of the measured change in the optical path length. The apparatus can accommodate both small and large working distances. For a microscopic field-of-view, the phase-shifted, laser feedback interferometer has been incorporated with an optical microscope.

This ATD consists of a multi-year effort to accomplish three specific goals: (1) build an interferometer based upon a continuous wave HeNe laser with stationary imaging optics and a translated sample, quantify the random and systematic measurement errors (including sensitivity to external perturbations) and calibrate the technique; (2) modify the two-dimensional scanning technique so that the sample remains stationary and the optics translate; and (3) develop a robust instrument which exploits LFI with semiconductor lasers.

Task Significance:

Often the primary science requirements of experiments of relevance to the Microgravity Science and Applications Division (MSAD), both ground-based and those requiring reduced gravity, involve the measurement of phenomena which can be evaluated by measuring the spatial variations of the path length of an interrogating light ray. These variations can arise either from changes in the index of refraction (a function of temperature, pressure, mass density, and concentration) along the path of the ray or from changes in the distance a ray travels.

Some examples of science requirements from experiments of relevance to the Fluid Physics and Transport Dynamics Discipline which can be determined from accurate measurements of the change in the optical path length include the determination of: (1) the location and orientation of a contact line and interface shape between two fluids; (2) the evolution of the thickness of a thin film; (3) deformation of a free surface due to evaporation or vibration; (4) resonant mode shapes in bubbles; (5) fundamental fluid parameters such as surface tension and viscosity; (6) variations in temperature and density in a fluid; (7) diffusion coefficients; and (8) fluid velocity.

The developed technology is likely to be attractive to many users outside the aerospace community. In fact, LFI will augment the ubiquitous uses of interferometry which have demonstrated applicability to nearly every scientific discipline including: physics, material science, mechanical engineering, chemistry and biomedical sciences.

Progress During FY 1996:

The first goal of the project has been achieved; a laser feedback interferometer has been constructed and calibrated by measuring the cantilever bending of a piezoelectric bimorph; static bending of less than a nanometer has been

II. MSAD Program Tasks — Advanced Technology Development

observed. This instrument has also been used in fringe counting mode to measure several microns of displacement. The systematic and random errors have been quantified. This instrument uses phase shifting techniques to simultaneously measure the change in optical path length and the fringe modulation. A model has been developed which predicts the response of the interferometer for samples with varying reflectivity (fringe modulation).

To improve the spatial resolution, a second phase-shifted interferometer has been incorporated into an optical microscope. This instrument incorporates piezoelectric stages to scan the sample underneath fixed optics. The instrument has been tested by measuring the three dimensional surface profiles of static liquid drops. The determined static contact angle of small drops of silicone oil on a coated surface of single crystal silicon agrees with measurements by other investigators.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/94 EXPIRATION: 9/98

PROJECT IDENTIFICATION:

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Proceedings

Ovryn, B., Eppell, S.J., Andrews, J.H., and Khaydarov, J. "Application of phase shifted, laser feedback interferometry to fluid physics." Proceedings of the Third Annual Microgravity Fluids Conference, Cleveland, Ohio, June 1996.

Presentations

Ovryn, B., Andrews, J.H., and Eppell, S., "Phase-measuring laser feedback interferometry: applications to microscopy." SPIE Vol. 2655, pp 153-163, 1996.

Ovryn, B., Andrews, J.H., Eppell, S., and Khaydarov, J., "Phase-shifted, real-time laser feedback interferometry." SPIE Vol. 2860, pp 263-275, 1996.

II. MSAD Program Tasks — Advanced Technology Development

Crystal Growth Instrumentation Development: A Protein Crystal Growth Studies Cell

PRINCIPAL INVESTIGATOR: Dr. Marc L. Pusey

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The goal is to design and construct prototype cells and a fluids preparation system for use in the study of the growth process of protein crystals. The cells should allow optical access for the study of the crystal growth process by a variety of techniques. Two cell designs are proposed. The first and most important will be for studies of the solution concentration gradients surrounding a growing crystal. The second design will be to study interfacial features of protein crystals under growth and etching conditions. A second goal of the proposed work will be to develop practical methods for protein storage prior to use in crystal growth (and other) experiments. The characteristics desired for a Protein Crystal Growth Analysis Chamber system for μg growth studies are:

1. Several types of growth cells to accommodate specific study goals.
2. Temperature control of the growth cell from 0 - 40 °C (± 0.05 °C).
3. Control of nucleation and growth of crystals at a defined location.
4. A fluidic system to accurately prepare crystal growth solutions from stock solutions of protein, precipitant, buffer, etc. and deliver them to the growth cell.
5. The cells should be accessible for additions to and/or modification of the solution.
6. The ability to do follow-up experiments based upon preceding growth runs.
7. Some cell adjustment to bring selected crystal faces in line (perpendicular or parallel) with the optical axes.
8. Easy accessibility to other solution measurement systems (pH, conductivity, etc.) for maximum data return.
9. Remotely operable from the ground to the maximum extent possible.
10. Ability to maintain proteins in a viable state prior to use.

Task Description:

Current microgravity (μg) protein crystal growth (PCG) hardware systems are hybrid, attempting to both acquire data about the processes of crystallization while growing crystals suitable for x-ray diffraction studies. This leads to compromises in the design, with the result that neither approach is successfully accomplished. The proposed hardware will be designed solely for studying the growth of protein crystals, which requires fewer experimental growth cells, but each having the maximum amount of data return and control of solution physico-chemical parameters.

A fluidics system able to prepare and simultaneously dispense two different solutions is now in the final stages of assembly. Upon completion, it will be connected to a crystal growth rate measuring system for functional testing. The final part of the assembly will be to add motorized translation stages for the positioning of the growth cell. The goal is to have all measurement operations done from the computer keyboard. The data obtained will be compared to that from previous measurements.

We will also be working on a means of storing protein solutions such that they remain viable, yet can be readily accessed by the fluidics system, during long duration (three months) μg missions. The results from an ongoing

II. MSAD Program Tasks — Advanced Technology Development

series of tests indicates that storage as a solution at 4 °C is most likely the best method for most proteins likely to be used as model materials for protein crystal growth. These tests involve the storage of proteins in two forms (in solution or as a freeze-dried powder) at three different temperatures (20 °C, 4 °C, and -20 °C). At periodic intervals the stored material will be sampled and tested for changes in crystallizability, turbidity, and if needed structural and functional integrity.

Task Significance:

In usage on board an orbiting platform ground-based researchers will be able to monitor and change selected solution parameters within the growth cells, and conduct follow-on experiments based upon recently acquired data. This will enable the realistic studying of how μg affects the protein crystal growth process, and how it can be improved both in space and on Earth. Long-term protein solution storage and stability will become a dominating concern as the time scale of g experiments increases. Developing methods for long-term protein storage will improve both this and future g -based instrumentation.

Progress During FY 1996:

With the recognition that higher performance interferometry systems would enable us to achieve all of our study's goals with smaller crystals and growth cells, we have now settled on small volume glass cells (0.3 mm x 10 mm x 30 mm) which have proven very suitable in routine use in an optical face growth rate measuring system in this laboratory. Solution temperature control will be developed along two lines. The first will be to stick with the now-developed method of surrounding the growth cell with a heater working against a surrounding cooling system. However, this method is very bulky, and adequate optical access to the growth cell may introduce thermal gradients across the cell with uncertainties about the actual temperature. These difficulties have led us to investigate the possibility of having a growth cell with a surrounding water jacket, with temperature control supplied by a remotely located circulating bath. This has the advantages of reducing the overall bulk of the growth cell, while enabling us to "dump" the waste heat from the regulation system elsewhere. This system will be exactly analogous to the most commonly employed temperature control methods in the laboratory.

The fluidics system has been reconfigured to improve its compatibility with the protein crystal growth cell. The redesigned system has two pairs of solution delivery syringes. Each pair is capable of independently preparing a solution, with the components being drawn from one of eight or more stock solution reservoirs. By going to this type of design, we are able to separately prepare the buffer and protein solutions, and mix them immediately prior to injection into the growth cell. The second syringe in each pair is used to allow the solution to be passed back and forth for mixing. Tests with a concentrated poly ethylene glycol and dye solution have shown that mixing can be achieved by this technique in the laboratory.

Two sets of long term storage stability measurements have been made using the proteins lysozyme and ovostatin. Storage conditions were at 20 °C, 4 °C, and -20 °C, both as a solution and as a lyophilized powder. The storage period was 3 months, and the materials were assayed for crystallizability every two weeks over this period. As expected, the least stable storage conditions were solutions at 20 °C. While lysozyme was expected to show exceptional stability, ovostatin was expected to be very sensitive to the storage conditions. Surprisingly, ovostatin showed a high degree of stability, as determined by crystallizability, both in solution and lyophilized at 4 °C, and the protein kept its crystallizability considerably longer than expected at 20 °C. We are now defining crystallization conditions for four new test proteins, lactate dehydrogenase, α -amylase, ovalbumin, and ovotransferrin, for use in storage (and other crystal growth) experiments over the next year. It should be pointed out that the lactate dehydrogenase being used was obtained over three years ago, and has been stored all this time as a suspension in 3.2M ammonium sulfate solution at 4 °C. This material is still pure by electrophoretic measurements and still crystallizes.

Together with William Witherow (NASA MSFC) and Alex McPherson (Univ. of California, Riverside), we responded to the glove box solicitation with a proposal to build a miniature interferometer and use it for protein crystal growth studies. This laboratory's contribution to the overall effort was to provide suitable growth cells and an associated fluidics system for providing the crystal growth solutions. Concurrent with this, we are now assembling a phase shift interferometer in our laboratory which will be connected to the completed fluidics system and used to verify its performance as well as ground-based data for comparison with the (future) μg experiments.

II. MSAD Program Tasks — Advanced Technology Development

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 2
MS Students: 0
PhD Students: 0

TASK INITIATION: 10/94 EXPIRATION: 10/96

PROJECT IDENTIFICATION: 963-70-02

RESPONSIBLE CENTER: MSFC

High Resolution Thermometry and Improved SQUID Readout

PRINCIPAL INVESTIGATOR: Dr. Peter Shirron

NASA Goddard Space Flight Center (GSFC)

CO-INVESTIGATORS:

DiPirro, M.J.

NASA Goddard Space Flight Center (GSFC)

Task Objective:

The objective of this work is to develop two technologies which are becoming increasingly central to low temperature microgravity research: high resolution thermometers and Superconducting Quantum Interference Devices (SQUIDs). A penetration depth thermometer (PDT) which uses thin film superconductors is being developed which can achieve nanoKelvin temperature resolution, similar to existing high-resolution paramagnetic salt thermometers (HRTs), while offering much greater flexibility in experiment design and immunity to particle radiation. Advanced SQUID sensors have been manufactured with far better intrinsic energy resolution than commercially available sensors. These sensors use a second stage array of 100-200 SQUIDs to amplify the signal from a single input SQUID. SQUID arrays and control electronics have been developed and are being evaluated for use in spaceflight applications.

Task Description:

The two efforts mentioned above have until now proceeded along independent paths. The emphasis during FY95 for the PDT development was to fabricate superconducting films with a transition temperature (T_c) in the range of 2.3-2.4 Kelvin. This would result in a thermometer with peak sensitivity at 2.17 Kelvin and make it suitable for use in both microgravity and ground-based studies of the lambda transition in liquid helium. Different geometries and film deposition techniques have been explored to determine which factors most significantly impact the sensitivity and noise of a thermometer. Measurements of temperature sensitivity and intrinsic resolution have been made using commercial SQUID system. The emphasis for the SQUID development has been the fabrication of flight quality control electronics and the continued evaluation of SQUID array chips which have been supplied by HYPRES, Inc. System level measurements of noise, power dissipation, bandwidth, and sensitivity to operating temperature and external magnetic fields are underway. Following this evaluation, the SQUID array system will replace the commercial system for reading out the PDT sensors.

Task Significance:

When studying critical phenomena (for example, the lambda point of liquid helium), the focus is usually on how certain parameters such as density or heat capacity vary with temperature close to the critical point. It is crucial for such experiments to determine or control the thermodynamic state to very high precision. Particularly in the microgravity environment, the precision to which temperature and/or pressure can be measured sets the limit for science return. Advances in current state-of-the-art for thermometry and SQUID sensors therefore translate into improvements in the quality of microgravity experiments. The SQUID technology will be particularly beneficial since SQUIDs have a wide range of uses, both in spaceflight applications and in ground-based laboratories. The PDT concept also can be adapted to allow non-contact temperature measurement. By not physically contacting the sample, parasitic heat inputs are minimized (important for heat capacity measurements) and mechanical dissipation is eliminated.

Progress During FY 1996:

- PDT sensors that operate near 2.17 K have been manufactured, with intrinsic temperature resolutions of 0.3 nanoKelvin/ $\sqrt{\text{Hz}}$. This represents a factor of 3 improvement within the last year. In the low frequency limit (<0.1 Hz) where most critical point experiments are conducted, this device is capable of detecting changes in temperature of 0.1 nanoKelvin.
- A high stability thermal platform for testing PDTs was constructed to allow testing while the PDTs are immersed in superfluid helium. This is essential, since in vacuum statistical thermal fluctuations ("thermal noise") is much larger than the resolution of the PDTs. The superfluid possesses such a large thermal conductivity and heat capacity that thermal noise is reduced to nearly negligible levels. The apparatus incorporates a pneumatically-actuated valve to allow a reservoir to be filled with superfluid, then thermally isolated from warmer stages.

II. MSAD Program Tasks — Advanced Technology Development

- Control electronics for the SQUID arrays with a "flux-locked loop" feedback circuit have been fabricated and tested. The overall system performance for the two-stage SQUID arrays and the electronics is $2 \text{ pA}/\sqrt{\text{Hz}}$ at frequencies above 300 Hz, and a bandwidth for small signal amplitudes of near 10 kHz. The noise figure is more than a factor of two better than the design goal. Below 300 Hz, however, the SQUID arrays themselves exhibit $1/f$ noise. Recent redesign efforts at reducing this excess noise have not succeeded. At present, the use of these SQUID devices is limited to applications in which the signal frequencies of interest are above several hundred Hz (for example, second-sound detectors for superfluid helium studies).
- A concept for multiplexing of SQUIDs has been developed and is being implemented. For applications requiring many SQUID readout channels, this multiplexing will allow the use of a single output array with multiple input SQUIDs. The advantage is a reduction in the number of excitation current and signal leads (a critical consideration for low temperature experimentation in space), and a simplification of the control electronics.

STUDENTS FUNDED UNDER RESEARCH:

BS Students: 0
MS Students: 0
PhD Students: 1

TASK INITIATION: 9/93 EXPIRATION: 9/97

PROJECT IDENTIFICATION: 963-70-70

RESPONSIBLE CENTER: GSFC

Passive Free Vortex, Two-Phase Separator

PRINCIPAL INVESTIGATOR: Dr. J. M. Shoemaker

Aerospace Design and Fabrication, Inc.

CO-INVESTIGATORS:

Schrage, D.
McQuillen, J.
Motil, B.

Aerospace Design and Fabrication, Inc.
NASA Lewis Research Center (LeRC)
NASA Lewis Research Center (LeRC)

Task Objective:

The primary objective is to develop an on-orbit fluid handling device to perform continuous gas-liquid separation using a low-power, passive free-vortex separator for phase accumulation and off-design operation, such as start-up or variable gravity environment. A separator that operates continuously will reduce the volumes required for both the liquid and gas phase used during operation of experiments over long periods of time. The goal is to develop and demonstrate the feasibility of a device applicable to two-phase experiments that uses very low power levels. The device would be an enhancement of the existing microgravity aircraft phase separator, expanding its utility, and will overcome the limitations of active, powered separator devices.

Task Description:

The existing KC-135/DC-9 Two-Phase Flow Rig will be utilized to conduct the experimental work. The Mod-0 development and testing effort is based on using the separator that is currently installed in the Two Phase Flow Rig and will include a series of modest improvements or changes to assess the performance characteristics. The development of the Mod-1 separator will be based on data collected and operational characteristics of the Mod-0 separator determined from previous flight tests.

Data obtained from the experimental testing of the Mod-0 separators and ground-based low gravity two phase flow rigs will be used to verify and refine the model for liquid film thickness, hydrostatic pressure rise, and liquid carryover. Analytical models will be developed to capture the fundamental physical behavior of the separators. The models will predict liquid film thickness, liquid flow rate, droplet trajectories, stability regions, and liquid carry-over based on the input of liquid flowrates, gas quality, and separator geometry. The performance models will be used to develop separator design software. The software will represent an optimization algorithm. Experimental data will be used to validate the models.

The analytical models will be used to design the next generation, Mod-1, of vortex separators. The Mod-1 will be built to determine flow characteristics and performance data which will be used to verify and refine the model. The performance models will be used to develop separator design software. Mod-1 vortex separator design will be based on the results of the analytical models developed in Task 1. Depending on the results, this design may incorporate an active drainage control feature. This feature would permit the control of the liquid drainage flow which would permit the gathering of data on the control and stability of the liquid film thickness on the wall. Control of the liquid film thickness is crucial in controlling the amount of liquid carry-over in the gas outlet stream and gas entrainment in the liquid outlet stream.

The next generation of separator, Mod-2, will include features for both liquid and gas closed-loop recycle. This task will provide for the development and testing of a breadboard liquid extraction system for use by the Mod-2 separator as well as the liquid drainage system. The liquid extraction system will be developed and tested. Also, any associated control system will be tested. The TPF Rig may be used to provide controlled two-phase flow for breadboard testing.

Task Significance:

The purpose of this study is to achieve a better understanding-better predictability-of two-phase (gas-liquid) flow in pipes to assist in the design of space-based power and thermal management systems and of the terrestrial-based nuclear power plants and oil and natural gas pipelines. Hydrocyclones are used as a means of gas-liquid separation in normal gravity, but have had very marginal success in their application in space-based systems.

II. MSAD Program Tasks — Advanced Technology Development

Progress During FY 1996:

Two flight series were conducted aboard the NASA LeRC DC-9 aircraft using the Large DC-9/KC-135 Two Phase Flow Rig. The first test series, conducted in April 1996, used the separator arrangement internal to the existing two phase collector/separator tank. Four single outlet injectors, consisting of tubing bent to redirect the entering flow tangentially replaced the multiple-orifice injectors that had a tendency to cause foaming. In addition, two chamber diameters, 23 cm and 30 cm, were used. Results indicated that the new injectors reduced the amount of foaming, and thus, the amount of liquid carryover in the gas outlet stream. There was no noticeable effect of chamber diameter on separator performance; however, flow visualization was hampered by several problems including leakage of the two phase mixture into an area in the separator tank that obscured the visualization.

The second test series was conducted in June 1996 and used an external separator preceding the existing two phase collector/separator tank. The new separator had a 15 cm. diameter. A vortex core was established and maintained for high flowrates. Slow flows could not generate sufficient momentum to start the vortex or even maintain it for the relatively short low gravity periods available aboard the aircraft. This separator concept is being modified for further investigation.

Analytical modelling of the phenomena is continuing and is being used to direct some normal gravity testing for bubble trajectory prediction. A separate, smaller test loop is being built for testing.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 2/96 EXPIRATION: 2/99

PROJECT IDENTIFICATION: 963-70-0L

RESPONSIBLE CENTER: LeRC

Determination of Soot Volume Fraction Using Laser-Induced Incandescence

PRINCIPAL INVESTIGATOR: Dr. Randall L. Vander Wal

NASA Lewis Research Center (LeRC)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

This project will develop a laser-based optical diagnostic technique, laser-induced incandescence (LII), for the measurement of soot volume fraction. The major objectives are to obtain the hardware and choose a combustion system of interest that yields relatively high soot concentrations, verify and develop the technique in the laboratory, including establishing LII on a quantitative basis, demonstrate LII in a laboratory flame under a variety of conditions and geometries, conduct reduced-gravity tests with LII and other complementary optical measurements, and assess the usefulness of LII as a measure of soot volume fraction.

Task Description:

We intend to develop laser-induced incandescence (LII) as a two-dimensional imaging diagnostic for the measurement of soot volume fraction for microgravity combustion research. LII, in conjunction with other optical imaging techniques, would provide unparalleled temporal and spatial resolution, and therefore, yield insight and sensitivity into soot formation and oxidation processes. Present methods of measuring soot volume fraction are limited to line-of-sight methods. These methods offer poor temporal and spatial resolution and require assumptions about the path length and soot physical properties. LII utilizes the spatial and temporal properties of pulsed laser excitation to heat soot to far greater temperatures than ordinary flame temperatures and exploits the resultant blue-shifted incandescent emission from the laser-heated soot. The incandescence is predicted theoretically to be a measure of soot volume fraction, which is the feature of soot that governs many physical processes such as radiative heat transfer from flames. This technique will be extended to two-dimensional imaging applications and will be calibrated against gravimetric sampling.

Task Significance:

Successful development of this diagnostic technique will provide detailed data on soot formation, growth, and oxidation processes for a variety of combustion systems, which may lead to a better understanding and control of sooting processes in flames.

Progress During FY 1996:

Tasks 1-2. Determine optimal signal detection strategies and minimize potential aggregate size effects: Experimental LII measurements were performed in a laminar gas-jet flame to test the sensitivity of different LII signal collection strategies and potential variations due to particle size. From experiments, we concluded the following: to prevent introducing a primary particle size dependent and/or local temperature bias in the LII signal, signal integration beginning with the excitation laser pulse is necessary. Signal integration times extending to 25 or 100 nsec after the laser pulse do not produce significant differences in radial profiles of the LII signal due to primary particle size and/or local gas temperature dependent cooling effects. Longer signal integration times extending hundreds of nanoseconds or signal integration times delayed from the excitation laser pulse reveal a decreased sensitivity to smaller primary particles or to similar sized particles in lower local gas temperature regions. While long wavelength detection reduces the sensitivity of the LII signal to these effects, only prompt detection of the LII signal beginning with the excitation laser pulse can effectively eliminate a primary particle size bias in the LII signal over the range of primary particle sizes and temperature variations encountered in an ordinary gas-jet diffusion flame. Finally, excitation of LII using 1064 nm light is recommended to avoid creating photochemical interferences thus allowing LII signal collection to occur during the excitation pulse without spectral interferences.

Task 3. Conclude whether theoretical analysis of LII is valid:

The effect of the high intensity laser light upon the soot was investigated through both normal and high-resolution transmission electron microscopy (TEM), selected area electron diffraction (SAED) and electron energy loss spectroscopy (EELS). The TEM allowed visualization of morphological changes in the laser-heated soot. The

II. MSAD Program Tasks — Advanced Technology Development

SAED and EELS techniques complimented the HRTEM to reveal the extent of molecular level changes in the laser-heated soot.

The observed changes such as formation of shell-like and rosette structures are similar to those observed in heat-treatment studies of carbon black. Visual inspection of the HRTEM images indicates extensive graphitization occurring as corroborated by the SAED patterns. While laser intensities ($< 1 \times 10^8 \text{ W/cm}^2$ @ 1064 nm) induce morphological changes in the primary particles, significant carbon mass loss apparently does not occur. Although theoretical models of LII do not predict the observations presented here of the effect of heating the soot, experimental measurements to-date confirm the validity of LII for providing a measure of the soot volume fraction. As LII provides a relative measure of soot volume fraction, the observed morphological changes likely result in a different relative value being measured. Given the observed morphological changes, agreement between theoretical predictions of the LII signal dependence upon primary particle size, laser intensity, wavelength, etc. and experimental observations must be cautiously interpreted.

Task 4. Conduct measurements under reduced pressure:

These measurements were performed in the variable pressure chamber. In collaboration with Prof. Mun Y. Choi (University of Illinois at Chicago) fiber supported droplets were studied. LII measurements were used to track the change in the soot spatial distribution and concentration with decreasing pressure. LII tracked soot volume fraction to levels more than three orders of magnitude below levels detectable via light extinction ($\sim 0.01 \text{ ppm}$) for fiber supported burning droplets of decane in 1-g. The comparison was based on fiber-supported burning droplets of toluene and decane.

Task 5. Combine LII images with other planar images:

LIF detection of polyaromatic hydrocarbons (PAHs) and LII measurements of soot have been performed in both spatially integrated and spatially resolved imaging measurements. Spectral emission scans present a fundamental step in identifying photochemical interferences which can interfere with LII or LIF measurements. Comparison of two-dimensional laser-induced emission images using either 1064 nm or 266 nm light allowed unambiguous spatial identification of PAHs and soot. Photophysical considerations suggest that 1064 nm light is unable to excite ultraviolet or visible fluorescence from PAHs except via an unlikely multiphoton excitation. Spatially resolved images using 1064 nm light indicate that this wavelength also does not produce other photochemical interferences and thus is ideal for inducing LII. The annular location of the laser-induced emission signal using 1064 nm excitation and long emission decay time constant is consistent with LII. Conversely the emission observed near the axial region with a short emission decay time constant is consistent with LIF due to PAHs.

Optimization of simultaneous LII-LIF measurements is achieved with detection occurring during the laser pulse and resulting fluorescence decay. Detection of LII and discrimination against LIF of PAHs is readily achieved with delayed signal detection. Consideration of the photophysical properties of PAHs indicates that the fluorescence wavelength distribution depends upon the PAH size. Thus with appropriate spectral filtering, different-sized PAHs may be selectively detected. With fluorescence detection within different spectral intervals, spatial variations in the fluorescence intensities are observed within a gas-jet diffusion flame. This radial distribution in the PAH size is consistent with the initial stages of soot formation beginning with small PAHs, their transformation via reactive acetylenic addition and eventual transformation into soot. Simultaneous LIF-LII images also reveal dark regions separating PAH and soot containing regions that were attributed to the presence of soot precursor particles. The presence of soot precursor particles within this region is consistent with these structures bridging the gap between molecular versus particulate material in the soot formation process. The presence of these particles in this region was directly confirmed using TEM analysis of the thermophoretically sampled soot in this region.

Task 6. Reduced gravity implementation plan:

The 2.2 Sec Drop Tower has been selected as the laboratory for low-gravity demonstration of this technique. Because of a variety of constraints (e.g. size and weight limitations on the drop packages), the laser system will be remotely located at the top of the tower. To deliver the laser light, an optical fiber running between the laser and drop package will be used.

II. MSAD Program Tasks — Advanced Technology Development

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/93 EXPIRATION: 9/97

PROJECT IDENTIFICATION: 94-2

NASA CONTRACT NO.: NAS3-271

RESPONSIBLE CENTER: LeRC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Vander Wal, R. L., Soot precursor material: visualization via simultaneous LIF-LII and characterization via TEM. 26th Comb. Symp., (accepted 1996).

Vander Wal, R.L., Laser-induced incandescence: detection issues. Applied Optics, (in press, 1996).

Vander Wal, R.L., Identification of soot precursor material via simultaneous LIF-LII and characterization via TEM. Combustion Science and Technology, (accepted 1996).

Vander Wal, R.L. and Dietrich, D.L., Laser-induced incandescence applied to droplet combustion. Applied Optics, 34, pp. 1103-1107 (November 1995).

Vander Wal, R.L., Jensen, K.A., and Choi, M.Y., Laser-induced emission measurements of soot and polycyclic aromatic hydrocarbons within a gas-jet flame. Combustion and Flame, (accepted 1996).

Vander Wal, R. L., Zhou, Z., and Choi, M. Y., Laser-induced incandescence calibration via gravimetric sampling. Combustion and Flame, (in press).

NASA Tech Briefs

Vander Wal, R. L., Laser-induced incandescence measurements of soot concentration in post-combustion exhaust. NASA Tech Brief, (Laser-Tech Briefs, accepted 1996).

Vander Wal, R. L., Visualization of polycyclic aromatic hydrocarbons and soot via laser-induced excitation. NASA Tech Brief, (Laser-Tech Briefs, accepted 1996).

Vander Wal, R. L., Soot visualization via laser-induced incandescence. NASA Tech Brief, (Laser Tech. Briefs 1996).

Presentations

Vander Wal, R.L., "Laser-induced incandescence: characterization and applications ." 26th Symposium on Combustion, Naples Italy, July 28 - August 2, 1996.

Vander Wal, R.L., "Laser-induced incandescence: detection issues." Central States Section Meeting of the Combustion Institute, St. Louis MO, May 5-7, 1996.

Vander Wal, R.L., "Soot precursor material: location via LIF-LII and characterization via TEM." Central States Section Meeting of the Combustion Institute, St. Louis MO, May 5-7, 1996.

Vander Wal, R.L., Jensen, K.A., Zhou, Z., and Choi, M.Y., "Soot precursor particles and polycyclic aromatic hydrocarbons: visualization through simultaneous laser-induced incandescence and laser-induced fluorescence imaging in diffusion flames." Eastern States Section Meeting of the Combustion Institute, Worcester MA, October 16-18, 1995.

Patents

Patent Approved, U. S. Patent #: Undetermined Vander Wal, R.L., "A patent application entitled "Laser processing of nanophase material" based on morphological changes observed in the laser-heated soot was submitted January 1995."

II. MSAD Program Tasks — Advanced Technology Development

Ceramic Cartridges via Sintering and Vacuum Plasma Spray

PRINCIPAL INVESTIGATOR: Mr. Frank R. Zimmerman

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

No Co-I's Assigned to this Task

Task Objective:

The objective of this development work is to provide a manufacturing process for containment cartridges used in high temperature (1200 to 2000 °C) crystal growth furnaces. A thermal spray process is used to build up refractory metals and ceramics into a containment cartridge for high temperature, single crystal semi-conductor growth experiments. These plasma spray formed materials have been evaluated for mechanical properties, density, microstructure, and resistance to liquid metal attack.

Task Description:

A thermal spray process is being used to build up refractory metals and ceramics into a containment cartridge for high temperature, single crystal semi-conductor growth experiments. This process uses high energy plasma inside a low pressure (100-200 torr) inert environment to apply layers of material onto a removable mandrel. A variety of materials are being characterized and evaluated against a demanding set of requirements, including high service temperature (1700 °C), oxidation resistance, and resistance to liquid metal attack. Techniques to spray form refractory metals (tungsten, molybdenum, niobium, tantalum) and ceramics (alumina, boron nitride) are being developed in the Plasma Spray Cell at Marshall Space Flight Center.

Task Significance:

NASA's Crystal Growth Furnace (CGF) has flown on the United States Microgravity Laboratory (USML-1 and -2) missions to conduct single crystal growth work on a variety of semiconductor materials. These semiconductor crystals (GaAs, CdZnTe, HgZnTe, HgCdTe) are grown in quartz ampoules surrounded by insulation, thermocouples, and other instrumentation. The entire experiment is contained within a Sample Ampoule Cartridge (SAC), which facilitates handling and installation into the furnace. The SAC also functions as a containment system, which is required to protect the flight crew from the highly toxic materials used in these crystal growth experiments. If the ampoule containing the crystal growth material should rupture, these cartridges provide a necessary level of containment. The containment requirement is complicated by the fact that most of these crystal growth compounds are known to aggressively attack most common structural metals at furnace operating temperatures. Currently, these cartridges are made of materials which are attacked at rates that will not fully penetrate the cartridge within the duration of the experiment. For experiments of longer duration, a more chemically resistant material is required to assure no breach in the containment will occur. Regardless of the material used, the current manufacturing sequence is labor intensive, dependent upon product availability, and contains several fabrication steps and joining processes.

Progress During FY 1996:

Addition of 1-3% nickel to tungsten was found to improve VPS product ductility, and verified to resist attack by gallium. Nickel was shown to diffuse into tungsten matrix, eliminating concerns about local chemical attack.

Introduction of non-contact failure detection system into the VPS formed cartridge. Objective is to embed sensor in the cartridge that will reliably detect ampoule failure without interfering with the ongoing science.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 10/93 EXPIRATION: 10/95

PROJECT IDENTIFICATION: 963-70-05

RESPONSIBLE CENTER: MSFC

Advanced High Brilliance X-Ray Source

PRINCIPAL INVESTIGATOR: Dr. Daniel C. Carter

NASA Marshall Space Flight Center (MSFC)

CO-INVESTIGATORS:

Gibson, W.
Kumakhov, M.
Ho, J. (X. He)

State University of New York, Albany
I.V. Kurchatov Institute of Atomic Energy
NASA Marshall Space Flight Center (MSFC)

Task Objective:

The primary objective of this research is to produce the first x-ray generator and Kumakhov lens system optimized in design for 8.0 KeV x-rays.

Task Description:

The x-ray unit will be integrated with existing x-ray diffraction equipment at Marshall Space Flight Center to produce a diffraction facility with the most advanced laboratory x-ray source for application in crystallography in the world. The approach to complete the task will be to produce intense small cross section parallel x-ray beams for structural analysis using third-generation Kumakhov optics.

Task Significance:

Protein crystallography is currently the most powerful method for the determination of the three-dimensional structure of proteins and other macromolecules. This method usually requires crystals which are relatively large in size and which possess a reasonably high degree of internal order. This research is concerned with the development of an extremely bright x-ray source for application in the evaluation and determination of the atomic structure of crystalline matter from both ground-based and current flight experiment activities.

Progress During FY 1996:

1. Advanced x-ray multicapillary optics have been successfully designed, constructed and evaluated by a team of scientists at MSFC, SUNY, and X-ray Optical Systems, Inc. to produce high intensity x-ray sources.
2. Initial tests of Stage II lenses surpass the original performance estimates and tests conducted in the MSFC Laboratory for Structural Biology indicate that the brightness of lens/x-ray source combinations should exceed by a factor of 160 those currently obtainable by a Rigaku RU200 rotating anode.
3. Low power systems operating at 37 watts have been demonstrated to exceed brightness of the current rotating anode generator by a factor of 2. The low power requirements and high brilliance of this prototype system have important implications for the development of a future orbiting diffraction facility on Space Station (i.e., feasibility has now been demonstrated), and in addition, also has applications in numerous other areas including medical imaging.

STUDENTS FUNDED UNDER RESEARCH:

TASK INITIATION: 4/93 EXPIRATION: 3/96

PROJECT IDENTIFICATION: 963-40-20

RESPONSIBLE CENTER: MSFC

BIBLIOGRAPHIC CITATIONS FOR FY 1996:

Journals

Ullrich, J.B., Huang, K.G., Owens, S.M., Aloisi, D.C., Hofmann, F.A., Gao, N., Klotzko, I.L., and Gibson, W.M. Concentration of synchrotron beams by means of monolithic polycapillary X-ray optics. Nucl. Inst. and Meth., vol. A364, 362 (1995).

Proceedings

Owens, S.M., Ullrich, J.B., Ponomarev, I.-Yu., Carter, D.C., Sisk, R.C., Ho, J.X., and Gibson, W.M. "Protein crystal structure measurements using polycapillary x-ray optics." SPIE Proceedings, vol. 2859-44, 1996.

Presentations

Carter, D.C. "Progress in the Utilization of Polycapillary X-ray Optics for Application in Macromolecular Crystallography." Gordon Research Conference, New Hampshire, June 1996.

Ulrich, J., Owens, S.M., Xiao, Q.-F., Ponomarev, I.-Yu., Carter, D.C., Sisk, R.C., and Gibson, W.M. "Convergent Beam Macromolecular Crystallography using Polycapillary X-ray Optics." International Union of Crystallography, Seattle, Washington, August 1996.

FY 96 INTER-AGENCY AGREEMENT

**NATIONAL INSTITUTE OF CHILD HEALTH AND HUMAN DEVELOPMENT
NATIONAL INSTITUTES OF HEALTH
and
OFFICE OF LIFE AND MICROGRAVITY SCIENCES AND APPLICATIONS
NATIONAL AERONAUTICS AND SPACE ADMINISTRATION**

The Microgravity Science and Applications Division (MSAD), Office of Life and Microgravity Sciences and Applications (OLMSA) of NASA, and the Laboratory of Theoretical and Physical Biology (LTPB), National Institute of Child Health and Human Development (NICHD) of NIH, are collaborating on a joint project in three-dimensional tissue culturing using the bioreactor technology developed by NASA. This agreement supports the transfer of ground-based NASA bioreactor technology for three-dimensional tissue culture to NIH and the external research community. Dr. Joshua Zimmerberg of the NICHD is the Director of the joint NASA/NIH biotechnology project and provides scientific and administrative supervision of the project. This agreement is effective through September 30, 1998, and may be modified by mutual consent of both parties. Peer review for continued funding of this project will be continuous and rigorous by the scientific counselors of the NICHD.

The National Aeronautics and Space Administration (NASA), through its Microgravity Biotechnology Program, has achieved a breakthrough in the engineering of tissues which allows for cellular growth, aggregation, and the development of *in vivo* like tissues. The National Institute of Child Health and Human Development (NICHD), through its Laboratory of Theoretical and Physical Biology (LTPB), is conducting biomedical research to elucidate the mechanisms of cellular dysfunction which lead to morbidity and mortality. Specifically, LTPB has developed a project on the long-term culture of human tissue for biomedical research. NASA and NIH have jointly focused their research and expertise on several fundamental medical science issues. This joint NASA-NIH program is using the unique talents and experience of both agencies to make a breakthrough in the culturing of human tissues for biomedical research. The first goal will be to engineer a human lymph node model for AIDS research. The second goal is to evaluate a broad spectrum of tissues available at the NIH.

Project Tasks

1. Create a core facility at NIH for the NASA bioreactor three-dimensional tissue culture technology, equipped to allow efficient growing of multiple cell types simultaneously, and staffed to provide technical assistance to visiting NIH and NASA investigators wishing to evaluate the new technology.
2. Develop tissue cultures for other NIH projects which require a higher level of organization than that available in monolayer or suspension culture by using the NASA bioreactor technology.
3. Augment the NIH three-dimensional tissue imaging facility to allow for critical measurements of intracellular calcium and pH in living bioreactor tissues, so as to judge tissue response to physiological and pathophysiological stimuli.
4. Grow cells obtained from human lymph tissue in the NASA Bioreactor, with full-time staff, and begin the development of an AIDS tissue model.

FY 1996 Annual Report

Executive Summary

In 1996, the NASA/NIH Center for Three-dimensional Tissue Culture became fully operational. Ten groups of intramural researchers from seven National Institutes, along with two extramural groups from Food and Drug Administration and Johns Hopkins University are funded for fundamental investigations that are of medical and biological importance. Of the 15 projects currently underway, four projects have significant results:

1. To understand formation of tissues and re-organization and differentiation of cells is one of the most important problems of Cell Biology. A new RWV-based system for formation of organized three-dimensional ductal acinar structures from disorganized aggregates of human salivary gland cells was recently developed at the NASA/NIH Center. In a static system developed previously, cells were affected both by physical factors, such as contact with a solid surface and by chemical factors (extracellular matrix). The new RWV system enabled researchers to discriminate between the effects of physical and chemical factors in the formation of gland structures: soluble extracellular matrix alone facilitated formation of acinar structures. In RWV, cells become more sensitive to cell-matrix interaction, and the formation of gland structures occurs in the presence of a lower amount of extracellular matrix than previously.
2. The main events in HIV pathogenesis occur inside lymphoid tissue connected *in vivo* by the recirculatory system with peripheral blood. To understand HIV pathogenesis, cultures of functionally active human lymphoid tissue were established using the RWV. This culture system supports productive infection with HIV-1, reconstitutes the recirculatory traffic of lymphocytes between lymphoid tissues, and enables HIV transmission between infected and non-infected tissues, allowing research on pathogenesis of giving the potential for rapid screening of therapeutics. Moreover, culturing of specific patient isolates of HIV resulted in differential death of intrinsic T cells which correlates to the known phenotype of each patient isolate. AZT, a leading anti-HIV drug, inhibits both viral replication and T cell depletion in our systems in a dose-dependent manner.
3. An experimental system to study epithelial metaplasia was established in the RWV bioreactor. The RWV system maintains a metaplastic phenotype in ductal human salivary gland tissue. The precise etiology and molecular changes associated with this pre-malignant condition disorder remain largely uncharacterized, partly because of the lack of a high fidelity *in vitro* system to study this disease. The RWV system will now be used to study the molecular changes associated with the transition of squamous esophageal metaplasia into overt dysplasia and eventual squamous carcinoma. The RWV system should also prove useful in studying potential therapies for this condition hoping to revert the metaplastic phenotype back into normal mucosa.
4. The RWV system maintained the tubuloglandular structure and stroma of human prostate tissue for at least five weeks of culture time. This has opened up several new directions for the study of the pathobiology of this clinically important tissue. RWV experiments are currently underway to test the hypothesis that prolonged alpha andrenergic stimulation can lead to benign prostatic hypertrophy. In conjunction with an ongoing NIH clinical study on hormone-refractory prostatic carcinoma, the RWV bioreactor has for the first time enabled this type of malignancy to be successfully cultured within a three-dimensional cytoarchitecture that supports the continued direct invasion of the stroma by the malignant cells. The RWV system also selectively amplifies the androgen independent stem cell compartment of the prostate, allowing study of gene regulation involved in the terminal differentiation of the glandular epithelium of prostate.

Each of these projects are the nucleus of a new class of investigations made possible by the Center. During the coming year we expect these projects to be augmented by others arising from the 11 other preliminary studies now underway.

I. SUMMARY

In 1996 NIH 10 groups of intramural scientists continued to work at the NASA/NIH Center for Tissue Culture on 14 various projects related to cell-cell interactions, cell differentiation and function, and crystal growth in NASA Rotating Wall Vessel Bioreactor. Four studies passed the Phase I stage of pilot projects. Those are projects on differentiation of salivary gland (Laboratory of Laboratory of Developmental Biology, National Institute of Dental Research), on metaplasia in human salivary glands and interactions of normal and neoplastic cells in human prostate (Department of Pathology, National Cancer Institute) and on HIV infection in human lymphoid tissue in vitro (Laboratory of Theoretical and Physical Biology, National Institute of Child Health and Human Development).

II. INTRODUCTION

This report outlines the activity of NASA-NIH Center for Three-Dimensional Tissue Culture in 1996. The Center was used by a number of scientists who work on projects related mainly to cell-cell interactions and cell differentiation, as well as infection with pathogens. According to our established procedures, in Phase I NIH scientists can launch pilot projects involving the RWV Bioreactor as extensions of their main intramural research projects. In addition, two projects were launched recently by extramural investigators from FDA and Johns Hopkins University. Based on these preliminary results an NIH group can apply for phase II, a small grant proposal of a study involving the RWV and get funding for purchasing RWV, disposables, as well as for post-doctoral fellow salaries. Four projects have now produced results beyond this preliminary phase:

1) *Differentiation of salivary gland cells in the RWV Bioreactor*, 2) *A model of the lymphoid system for studying HIV infection in vitro*, 3) *RWV Bioreactor models of human squamous metaplasia*, and 4) *Long term maintenance of human prostate explants in the RWV*.

Below are brief descriptions of the current projects at the NASA/NIH Center, by Institute.

III. PARTICIPATING LABORATORIES AND PROJECTS

NIDR

- 1) Differentiation of salivary gland cells in the NASA Bioreactor.

NICHD

- 2) Human lymphoid tissue in the NASA Bioreactor; A two-compartment model of the lymphoid system for studying HIV infection in vitro.
- 3) Human spleen, lymph node, and bone marrow; A three-compartment NASA Bioreactor based model for studying T-cell Differentiation and lymphocyte traffic.

NCI

- 4) NASA Bioreactor models of human squamous metaplasia.
- 5) Long term maintenance of human prostate tissue in the NASA Bioreactor.
- 6) NASA Bioreactor models of adenocarcinoma invasion/metastasis.

NIAID

- 7) In vitro hepatocyte infection by avian malaria in the NASA Bioreactor.
- 8) In vitro production of Herpes Zoster Virus using human skin explants in the NASA Bioreactor.

NCHGR

- 9) Use of the NASA Bioreactor to improve the efficiency of vector transfer in gene therapy protocols.

NIDDK

- 10) Protein crystal growth in the NASA Bioreactor.

FDA

- 11) Long-term three-dimensional culture of intestinal tissue in the NASA Bioreactor to study the interactions of bacteria and parasites.

NINDS

- 12) Long-term three-dimensional NASA Bioreactor culture of neonatal rat hypothalamus to study neurosecretory pathways.
- 13) NASA Bioreactor epithelial cell studies on the unknown molecular pathogenesis of Mucopolidosis Type 4 (ML4).
- 14) Differentiation of human dendritic cells in the NASA Bioreactor.

JOHNS HOPKINS UNIVERSITY

- 15) Use of the role of gap junctions in NASA Bioreactor to evaluate the lymphoid tissue function.

IV. INDIVIDUAL PROJECTS: PROGRESS REPORTS AND PLANS

1. Differentiation of salivary gland cells in the NASA Bioreactor.

Primary Investigators: Hynda Kleinman, PhD, and Matthew Hoffman, PhD, Laboratory of Developmental Biology, National Institute for Dental Research, NIH.

Aim of Experiments: To determine the ability of the Human Salivary Gland (HSG) ductal cell line to form three-dimensional salivary gland duct structures during RWV Bioreactor culture.

BACKGROUND:

During development, the intercalated ductal cells of the salivary tissue are thought to be pluripotent stem cells which eventually give rise to the acinar structures which characterize this tissue. The HSG cell line is derived from these ductal elements and when cultured on basement membrane extracts (Matrigel or Laminin-1) by regular tissue culture techniques, these cells have been shown to undergo acinar differentiation.

Experiment Design: HSG cells will be subjected to RWV Bioreactor culture both with and without the addition of Matrigel, laminin-1, or the LQVQLSIR peptide derived from Laminin-1 and assessed by histological appearance for the formation of acini or acini-like structures. Vital stains and confocal laser microscopy will be utilized to study the three-dimensional structure of any cellular aggregates which develop in this system.

Preliminary Results:

1. The RWV Bioreactor is able to support the growth of HSG cells for a minimum of one week. The cells form disorganized aggregates and do not polarize under the simulated microgravity conditions afforded by the RWV system.
2. HSG cells grown in the RWV Bioreactor with the addition of basement membrane extract (Matrigel), Laminin-1, or the Laminin-1 peptide LQVQLSIR, were observed to form organized three-dimensional spherical acinar-like structures which have polarity. In terms of polarization, the best results were observed in the Matrigel containing bioreactor.
3. The process of acinar formation within the RWV system was found to be both cell density dependent as well as dependent upon the concentration of the artificial matrix added to the bioreactor.

Plans: Over 700 short peptides from the laminin family of molecules have been assessed and of these, five peptides have been selected for further study in the RWV Bioreactor. We intend to look at both the morphology as well as certain biochemical aspects of salivary gland development; specifically, the role of the cystatin protein as a marker for salivary gland cell differentiation and the expression of laminin receptors in the RWV cultured cells. In addition certain signaling pathway studies are planned to determine if phosphorylation plays a role in epithelial cell differentiation in this tissue.

2. Human lymphoid tissue in the NASA Bioreactor; A two-compartment model of the lymphoid system for studying HIV infection in vitro.

Primary Investigators: Leonid Margolis PhD, and Joshua Zimmerberg, MD, PhD, LTPB, National Institute of Child Health and Development, NIH.

Aims of Experiment: HIV infects cells in a variety of body compartments. Although the main events in HIV disease occur in the lymphoid tissue, the homeostasis of the entire hematopoietic and lymphoreticular system becomes affected. The current hypothesis concerning the development of AIDS are based on an impaired interaction between the lymphoid tissue and the peripheral blood. In order to test these hypothesis, we are studying the pathogenesis of HIV using peripheral lymphocytes which interact with cultured human lymphoid tissue under controlled conditions in vivo.

Specifically our goals are:

1. To develop methods for re-supplying new lymphocytes to RWV cultured human lymphoid tissue.
2. To study the contribution of recirculatory traffic of HIV-infected peripheral lymphocytes to the pathogenesis of HIV infection in human lymphoid tissue.

BACKGROUND:

It has been established that the pathogenesis of HIV infection involves a complex interplay between both infected and non-infected cells of the human immune system, the release of free viral particles, *de novo* cell infection, and the recirculatory lymphocyte cell traffic associated with the peripheral blood. However, most studies of HIV infection have been performed with cell lines or suspensions of stimulated peripheral blood lymphocytes. A significant limitation of these current systems for studying the pathogenesis of HIV is the absence of an early progenitor cell compartment which can provide cultured lymphoid tissue with a continuous re-supply of lineage committed T and B-cells and macrophages, similar to the conditions in vivo. Therefore, to develop a high fidelity model of the human lymphoid system, it is necessary to develop a method to re-supply new lymphocytes to the cultured lymphoid tissue.

Experiment Design: The rotating wall vessel (RWV) bioreactor is a recently developed system designed to grow cells either in suspension under conditions which minimize the disruptive effects of mechanical shear. In our experiments last year we extended these applications to culture actual fragments of human lymphoid tissue, and we modified the RWV system into a two-compartment model by adding peripheral lymphocytes to the surrounding culture media. Various mixtures of HIV-infected and non-infected lymphoid tissue explants were placed into the RWV together with peripheral blood mononuclear cells (PBMC) and it was possible to compare the pathogenic effects of HIV when the infection started in the peripheral cells or when it was induced by free virus. By modulating the amount of peripheral cells re-populating the lymphoid tissue explants, it is now possible to experimentally test various hypothesis concerning the dynamics of HIV-infection and lymphocyte depletion.

Preliminary Results:

1. Fragments of surgically excised human lymphoid tissue (tonsil and lymph node), remain viable and retain their native cytoarchitecture for at least three weeks when cultured in the RWV system. The lymphoid tissue gradually shows a loss of both T and B cells from the tissue into the surrounding growth medium, however this cellular migration is reversible. Using confocal microscopy, we have shown that labeled cells in the peripheral medium are able to traffic back into the explanted lymphoid tissue blocks and take up residence.
2. When explanted lymphoid (tonsil) tissue blocks are co-cultured in the RWV with a continuous high density of PBMC in the surrounding culture media (2.9×10^7 cells/ml), there is a dramatic improvement in both the histological cellularity of the tissue, as well as the maintenance of a normal resident CD4+ / CD8+ lymphocyte ratio

after long duration culture. These observations further indicate that there is a high continuous rate of lymphocyte cell traffic into the RWV lymphoid tissue cultures, similar to the conditions found in vivo.

3. The improved cellularity afforded by this high density bioreactor system allowed for the first time, a measurement to be made concerning the rate of CD4+ cell depletion in cultures infected with the LAV strain of HIV-1. In accordance with the natural pathogenesis of HIV disease in vivo, prolonged RWV culture of LAV infected lymphoid tissue showed the progressive and complete depletion of the CD4+ lymphocyte subset. It is therefore reasonable to suggest that this high density RWV bioreactor model may be a useful for studying basic mechanisms of HIV pathogenesis in human lymphoid tissues.

Plans: To extend the applications of the high density RWV Bioreactor with respect to discerning the effects of lymphotropic/macrophage tropic strains, differing HIV clades, and the efficacy of various chemotherapeutic agents. Basic immunological features of HIV disease will also be studied, particularly CD8+ cell mediated immunity. The culture system will be further modified into a multi-compartment model with the addition of human lymph node explants and thymus tissue. HIV infection will be further studied in this system. This project will contribute not only to the basic science of cell-cell interactions but also to applied studies of HIV pathogenesis. Various hypotheses formulated on the basis of patient/isolate correlation's (mutations in the env and nef genes, long-term non-progressor's), can now be tested under controlled in vitro conditions using patient material and recombinant virus. Some aspects concerning the current models of T-cell dynamics in HIV-infected patients, can also now be tested in vitro.

3. Human spleen, lymph node, and bone marrow ; A three-compartment NASA Bioreactor based model for studying T-cell differentiation and lymphocyte traffic.

Primary Investigators: Steven Hatfill MD, PhD, Leonid Margolis PhD, LTPB, National Institute of Child Health and Development, NIH.

Aims of Experiment: Classical immunological thought outlines the thymus as the site for terminal T-cell differentiation and the deletion of self- immunoreactivity. While we agree with this concept for the perinatal and juvenile human, the histological involution of this organ with age leads us to hypothesize that in the adult, the major site of T-cell differentiation in the adult is the spleen. In order to test this hypothesis, we are studying a mixed type culture system which utilizes a fluidized bed bioreactor to maintain human bone marrow and provide precursor T-cells to an RWV based spleen, adult thymus, and lymph node culture system.

Specifically our goals are:

1. To facilitate the survival and preservation of the native three-dimensional cytoarchitecture of explanted biopsies of human bone marrow and its functionality with respect to the production of early T-cell precursors in a fluidized bed bioreactor.
2. To facilitate the survival and preservation of the native three-dimensional cytoarchitecture of human tissue explants of the spleen, tonsil and lymph node in the RWV Bioreactor during co-culture.
3. To study the traffic of T-cell precursors from the cultured bone marrow to RWV co-cultured explants of human spleen and adult thymus and to determine if double positive CD4+/CD8+ precursor cells can mature into separate CD4+ and CD8+ lymphocyte sub-populations within the spleen.
4. To determine if human bone marrow progenitor cells cultured in the fluidized bed bioreactor are capable of maintaining the normal B and T lymphocyte sub-populations in RWV co-cultured explants of human tonsil, lymph node and spleen and to study the kinetics of the lymphocyte traffic between these organs in vitro.

BACKGROUND:

Classical immunological theory holds that the human bone marrow is responsible for producing early T-cell precursors which then leave the marrow and traffic to the thymus gland where they undergo terminal differentiation into the various T-cell subtypes and are subjected to deletion to remove clonal cells which possess “self-reactive” T-cell receptors on their outer cell membranes. In the neonate and juvenile human, the thymus is a large and active organ. However, with advancing age the thymus regresses and in the adult, the amount of discernible lymphoid tissue in this organ is histologically minimal. It has been estimated that the adult bone marrow produces a constant number of lymphocytes per day. The high absolute numbers of T-cells circulating in the peripheral blood and resident in the lymphoid tissues, suggests that a large proportion of these newly produced lymphocytes should already be committed to the T-cell lineage. The relative absence of discernible lymphoid tissue in the thymus of adults compared to the abundance of thymic tissue in the neonate and juvenile, leads us to suggest that the major site of T-cell differentiation in the adult lies in an organ outside the thymus gland. Such a change of functional organ sites is not unusual in mammalian physiology. For example, for much of fetal life the mammalian liver is the major site of hematopoiesis and only after early development is finished, is this function shifted to the bone marrow. We hypothesize that the spleen is a major site for T-cell differentiation in later life and that the development of a high fidelity *in vitro* model of the adult human immune system should take this organ into consideration.

Experiment Design: The high density of human bone marrow biopsies precludes the possibility that this tissue can be cultured in the RWV bioreactor in a manner which preserves the native cytoarchitecture. The fluidized bed bioreactor (FBR) is a recently developed system for long duration murine bone marrow culture, which with slight modifications is applicable for long duration human bone marrow culture.

Trephine biopsies will be obtained as a byproduct of normal marrow donor work up, and subjected to FBR culture. Non-adherent cells are harvested from the marrow culture at weekly intervals in a sample volume of two ml and a small aliquot is characterized with respect to cell numbers, maturation, and differentiation. The remaining bulk of the cells are labeled with PKH-26-GL fluorescent membrane dye before they are introduced into the culture media of an RWV bioreactor which for the first experiments will contain only explants of human spleen. Later experiments will involve co-cultures of both human spleen and human thymus. The preferential ability of these precursor cells to home to the target organ explants in the RWV bioreactor will be assessed by confocal microscopy and FACS analysis. Cells will be shaken out of the individual tissue blocks over a 10 day time course and analyzed by FACS for the presence of double positive CD4+/CD8+ cells and the number of single positive CD4+ and CD8+ cells. Parallel RWV cultures of spleen and spleen/ thymus will be run without the addition of bone marrow precursor cells to the culture media. Histological methods using two recently developed monoclonal antibodies for CD4+ and CD8+ which work on paraffin sections, will be used to determine the precise location of these cells within the thymus and spleen cytoarchitecture. Following this initial characterization of the T-cell system, the experiments will be further extended with respect to the B-cell system using spleen, human lymph nodes, and tonsillar tissue cultured in the RWV bioreactor. Later experiments will involve removing selected blocks of spleen, lymph node and tonsil tissue and staining each with a different fluorescent marker. These stained tissue blocks are then reintroduced into the bioreactor to further study the traffic of lymphocytes and their relative residency times within these organs. The normal residency time of mature B-cells within the bone marrow is unknown. By introducing labeled cells from the RWV back into the FBR, we will attempt to estimate the kinetics of this process *in vitro*.

Preliminary Results:

1. Fragments of surgically excised human spleen and lymph node remain viable and retain their native cytoarchitecture for at least 2 weeks when cultured in the RWV bioreactor.
2. Initial experiments suggest that labeled cells shaken out of human tonsillar tissue can traffic into high density RWV cultured fragments of human spleen to take up residence in this tissue.
3. Labeled cells shaken out of human spleen can traffic into high density RWV cultured fragments of human tonsil to take up residence in this tissue.

4. Because of the high density afforded by the intermedullary trabeculae, the RWV bioreactor is unsuitable for culturing human bone marrow within the context of its native three-dimensional microenvironment. Construction of a modified fluidized bed bioreactor is complete and preliminary characterization of this system for long duration bone marrow culture is underway.

Plans: Experimental work will continue to characterize the ability of the fluidized bed bioreactor to support long duration human bone marrow cultures. At the same time, homing and differentiation experiments will be performed on RWV bioreactor cultured blocks of human spleen tissue, using purified and labeled double positive CD4+/CD8+ cells from human marrow aspirates added to the bioreactor culture media. HIV infection will also be studied in this system. This project will contribute not only to the basic science of lymphocyte trafficking and progenitor T-cell differentiation, but also to applied studies of HIV pathogenesis which concern HIV-infected lymphocyte sequestration.

4. NASA Bioreactor models of human squamous metaplasia.

Primary Investigators: Paul Duray, MD, Department of Pathology, National Cancer Institute, NIH.

Aims of Experiments: Metaplasia concerns the transformation of one adult cell type within a tissue into another cell type. In many instances, this transformation is thought to be a precursor to neoplasia and the genetic mechanisms responsible are poorly understood. We are utilizing the RWV bioreactor for genetic studies concerning the metaplastic phenotype of human epithelial cells within their native tissue microenvironment. We hypothesize that in some instances there is a successive progression from metaplasia to eventual dysplasia and invasive carcinoma, and that such irreversible metaplasia is associated with a loss of heterozygosity at the APC gene locus.

Specifically the goals are:

1. To determine if cells with a pre-existing epithelial metaplastic phenotype can be maintained within the context of an otherwise normal tissue environment during long duration RWV bioreactor culture.
2. To determine if cells with a pre-existing epithelial dysplasia can be maintained within the context of an otherwise normal tissue environment during long duration RWV bioreactor culture.
3. To determine if metaplastic epithelial cells in the RWV bioreactor can be experimentally made to undergo morphological changes consistent with dysplasia during culture.
4. To determine if a loss of heterozygosity at the APC gene locus is responsible for the irreversible progression of metaplasia into the dysplasia associated with Barrett's Esophagus.

BACKGROUND:

Barrett's Esophagus is the second most rapidly increasing cancer in western society and the cause and pathogenesis of this disease is unknown. Histological studies suggest there is a successive progression from metaplasia to dysplasia with eventual invasive adenocarcinoma, but there is no direct evidence that metaplastic epithelia are clonal precursors to this or other types of epithelial cancer. Recent studies have implicated APC gene alterations as one of the earliest genetic changes that occur during progression from a histologically benign to a malignant epithelial phenotype. Using the techniques of microdissection and the Polymerase Chain Reaction (PCR), it is now possible to investigate APC gene alterations in different histological regions of a tissue which are representative of the potential stages of progression from the metaplasia associated with Barrett's esophagus to dysplasia and overt carcinoma. In addition, this technology allows clonal studies to be performed to assess whether metaplasia, dysplasia, and carcinoma are derived from the same cellular origin. However, it is first essential to develop an in vitro model so that this process can be studied under controlled conditions.

Experiment Design: The RWV Bioreactor will be used to subject small blocks of several types of human tissue with a pre-existing metaplastic component, to long duration culture. The continued maintenance of the metaplastic component of this tissue during culture will be assessed by immunohistochemistry using a defined panel of epithelial-associated cell surface antigens and thin section histology. These experiments will serve to demonstrate the ability of the RWV bioreactor to maintain the metaplastic phenotype, and a number of different induction agents will later be added to the culture medium in an effort to induce histological dysplasia. In addition, specific surgically biopsied samples from patient's with Barrett's esophagus will be obtained under an approved NCI protocol and subjected to long duration RWV culture. Using microdissection and PCR techniques, metaplastic and dysplastic areas within the RWV cultured tissue will be assessed for APC heterozygosity and clonality.

Preliminary Results:

1. The RWV bioreactor was able to maintain a pre-existing metaplastic epithelial phenotype in a patient with sialometaplasia of the minor salivary glands and excretory ducts. This metaplasia was confirmed by immunohistochemistry and was maintained for the entire 11 days of the experiment in otherwise histologically normal human oropharyngeal tissue surround.
2. Three experiments have been run to date using surgically removed full thickness blocks of murine esophagus to define the conditions necessary for RWV bioreactor culture. These experiments have shown mixed results with respect to epithelial cell viability and refinement of the necessary culture conditions is continuing.
3. With respect to preliminary estimates of the RWV bioreactor to culture human tissue with dysplasia, three separate experiments have shown the ability of the RWV bioreactor to culture full thickness explants of human skin. This RWV cultured tissue was shown to be able to maintain an active and histologically normal basal cell layer, a stratified squamous layer with keratinization, intact hair follicles, and normal appearing melanocytes, for a minimum of 14 days of culture. These baseline experiments are now being extended in an attempt to culture dysplastic naevi in the RWV system.

Plans: Current studies suggest that the RWV bioreactor is capable of culturing at least one type of human metaplastic tissue, that of the minor salivary glands and excretory ducts. Work is continuing with a focus on defining the best culture media and size of the tissue explants with respect to dissected samples of murine esophagus. This data will be used to define the bioreactor culture conditions necessary for human esophagus tissue samples. The first surgical biopsies from patients with Barrett's esophagus are scheduled to begin arriving on 11/96. The RWV cultures will be extended to test the ability of various induction agents to transform this dysplasia into overt melanoma within the bioreactor. Upon the successful RWV culture of human esophagus, this melanocyte data will be used to select the best induction agent for an attempt to transform RWV cultured tissue from Barrett's esophagus patients into adenocarcinoma. Microdissection and molecular techniques will then be used to determine the clonality of this metaplastic-dysplastic-carcinoma progression.

5. Long term maintenance of human prostate tissue in the NASA Bioreactor.

Primary Investigators: Paul Duray, MD, Department of Pathology, National Cancer Institute, NIH.

Aim of Experiment: To utilize RWV Bioreactor technology to develop a long duration in vitro tissue model of the human prostate suitable for the investigation of prostatic epithelial pathobiology. The primary focus of these experiments is to develop a high-fidelity in vitro model of normal prostate tissue structure and function which is suitable for testing the hypothesis that certain pesticide residues may cause a disruption of normal prostatic function and that a loss of heterozygosity at the 8p12-21 locus is responsible for the invasive nature of primary prostatic cell carcinoma.

BACKGROUND:

Recent epidemiological data suggests a pronounced and unexplained increase in the incidence of prostatic carcinoma in the United States. The etiology for this increase is unknown and there is an urgent need for an accurate in vitro model of normal human prostate structure and function to test various hypothesis for this increased incidence and the genetic changes responsible for the transformation of prostatic intraepithelial neoplasia (PIN), into invasive adenocarcinoma. To date, the most widely used method for the culture of prostate tissue explants has been the raft histoculture technique. A major short-coming of this method is the requirement for the exogenous addition of insulin and androgen hormone to the culture media and the limited time that such cultures can be maintained with a normal histology.

The ability of the RWV Bioreactor to facilitate three-dimensional cell-cell and cell-extracellular matrix interactions makes this a likely culture system to attempt long duration epithelial cell maintenance in prostate tissue explants.

Experiment Design: Initial experiments will focus on the ability of the RWV Bioreactor to culture small blocks of benign human prostate tissue obtained as a byproduct of transurethral prostatectomy under an existing NCI protocol. Samples of the cultured tissue will be periodically removed from the bioreactor and subjected to thin section histological examination, immunocytochemistry for the presence of acid phosphatase and Prostatic Surface Antigen (PSE), and RT/PCR for PSA gene expression. The limits of the RWV system for this type of tissue culture will be explored with progressively longer bioreactor culture times and the ability of the system to culture tissue blocks which contain PIN. In addition, the cultured tissue blocks will be subjected to microdissection and PCR analysis to prove the feasibility for future genetic studies concerning the 8p12-21 locus.

Preliminary Results: The RWV Bioreactor is able to successfully culture surgically removed blocks of benign human prostate tissue for up to five weeks of continuous culture time. These experiments have shown the unexpected ability of the RWV bioreactor to maintain normal appearing tubuloglandular epithelium without the need for exogenous insulin or androgen supplementation to the culture media. The prostatic epithelial cells maintain both a normal polarity and height and there is evidence for their continued secretory function throughout the duration of culture.

2. The stromal elements of the RWV cultured blocks of human prostate appear to increase in complexity and cellularity after the initial first week of RWV culture. This stromal reorganization continues for approximately 3 weeks.
3. The secretion of Acid Phosphatase by the prostatic epithelial cells is maintained throughout 5 weeks of RWV culture time. Prostatic Surface Antigen expression is down regulated at roughly the same time that stromal re-population of the tissue blocks is observed to occur. This suggests the presence of a possible regulatory interaction by the prostate stroma on PSA expression.
4. The use of 99% ethanol/ 1% glacial acetic acid as a fixative, permits DNA to be easily cultured prostate tissue. This DNA appears suitable for a variety of PCR and RT/PCR studies concerning PSA and androgen receptor expression, as well as heterozygosity extracted from microdissected thin tissue sections prepared from the blocks of RWV studies for loci on chromosome 8.

Plans: Current studies suggest the RWV bioreactor is capable of culturing human prostate tissue for a minimum of 5 weeks. Work is continuing with respect to identifying the effects of exogenous androgen administration to this RWV cultured tissue and the ability of this system to culture tissue blocks containing PIN. When these studies are complete, a series of experiments will be performed to assess the effects of a number of environmental estrogen mimicking agents on RWV prostate tissue blocks. These agent include; the polychlorinated biphenyls, nonylphenols and bisphenol-A. Separate experiments are being designed with respect to using the RWV system to elucidate the possible role of the 8p12-21 loci in prostatic metastatic cell transformation.

6. NASA Bioreactor models of adenocarcinoma invasion/metastasis.

Primary Investigators: Paul Duray MD, Dept. Of Pathology, National Cancer Institute.

Aim of Experiments: The “seed and the soil” concept in tumor biology refers to the propensity of certain human tumors to undergo preferential metastasis to a limited number of specific organs. The biochemical reasons for this remain largely unknown. The lack of gravity induced sedimentation afforded by the RWV Bioreactor makes this an ideal culture system to study the microenvironment in which host extracellular matrix and tissue cells interact with infiltrating metastatic tumor cells.

Specifically our goals are:

1. To determine if the RWV bioreactor can support the metastatic spread of human tumor cells into cytoarchitecturally normal human tissue.
2. To determine if the RWV bioreactor can support the metastatic spread of human tumor cells into cytoarchitecturally normal murine organ explants.
3. To utilize immunohistochemical methods to determine if the metastatic spread of human tumor cells involves the expression of different matrix metalloproteases in different target tissues.
4. To use PCR based subtractive hybridization to identify possible target genes responsible for the differing target organ tropism in metastatic subtypes of prostatic carcinoma.

BACKGROUND:

It has been long realized that certain malignant tumors have a specific propensity to metastasize to certain target organs. This is evidenced by the ability of bronchial carcinoma to metastasize to other areas of the lung and brain, breast cancer to metastasize to the lymph nodes, and prostate cancer which demonstrates a differential ability to metastasize to either the bone marrow, lymphoid tissue, or lung. This phenomenon is often referred to as the “seed and the soil” concept whereby the metastatic cells (the seed) have a preferential ability to home to a specific distant target organ (the soil). The molecular mechanisms responsible for this selective metastasis are undefined but probably involve a complex interplay of cell adhesion molecules, matrix receptors, metalloprotease enzyme secretion and local microenvironment. Identification of the factors involved in this process could lead to novel approaches in the clinical management of metastatic disease.

Experiment Design:

The RWV Bioreactor will be used to subject small blocks of normal human and murine lung and lymph node to long-duration co-culture with both a primary bronchial carcinoma cell line and explants of human bronchial carcinoma tissue obtained under an existing NCI protocol with the National Naval Medical Center. These experiments will focus on the ability of the RWV system to support metastatic spread of human carcinoma cells into normal human and mouse lung tissue and lymph node. Co-culture experiments will also be performed using the TSU metastatic human prostate cell line and explants of both normal and malignant prostate biopsy material and normal human lymph nodes obtained through an existing NCI protocol. This culture system will then be used to determine the degree of expression of the matrix metalloproteases in the metastatic cells of the co-cultured lymph nodes and the local invasion of the primary host tissue. These metalloproteinases include; Collagenase-3, Gelatinase-A and B, Stromelysin-1 and 2, Matrilysin, and Metalloelastase. If the co-culture experiments using human cell lines and mouse target tissue are successful, experiments will be done using a PCR based subtractive hybridization assay to identify genes responsible for variable metastatic target tissue tropism in human bronchial carcinoma, and human prostate adenocarcinoma.

Preliminary Results:

1. The RWV Bioreactor is able to support the growth and invasion of human squamous bronchial carcinoma into normal co-cultured explants of normal human lung tissue.
2. The RWV Bioreactor is able to support the growth and local invasion of TSU prostate carcinoma cells into co-cultured explants of both normal human lymphoid tissue and normal human prostate. The cells are seen to attach to the explanted tissue blocks where they invade and destroy the normal tissue cytoarchitecture.
3. Preliminary experiments have been performed using a fluidized bed bioreactor for bone marrow culture to add this component to the experimental metastatic RWV system.
4. A variety of mouse organ explants have been cultured in the RWV bioreactor; these include liver, spleen, lymph node, lung, thyroid, and parathyroid glands. These explants have been successfully co-cultured within a single RWV bioreactor for a minimum of 7 days. Difficulties have been noted for RWV cultures of mouse brain, kidney, pancreas, retina, stomach, and small bowel and refinements of the culture system for these organs are being considered.

Plans: Work will continue on co-culturing malignant human lung and prostate cell lines and studying the pattern of matrix metalloproteinase expression during the invasion of normal human tissue explants in the RWV. The spread of prostatic carcinoma in the fluidized bed bone marrow bioreactor will also continue to be defined with respect to the ideal culture conditions for this system. Multi-system mouse organ co-cultures will be used to define the ability of the RWV system to detect the metastatic tissue tropism of malignant prostate cells from the biopsies of individual patients. This material will also be subjected to metalloprotease analysis and later microdissection, PCR and subtractive hybridization using malignant prostate cells from different patients with differing metastatic tissue tropisms.

7. In vitro hepatocyte infection by avian malaria in the NASA Bioreactor.

Primary Investigators: Helmut Ziegler PhD, National Institute of Allergy and Infectious Diseases, Laboratory of Parasitic Diseases, NIH.

Aim of Experiment: To utilize RWV Bioreactor technology to develop an in vitro system capable of supporting *Plasmodium* sp. malaria parasite development in the vertebrate liver and mosquito midgut.

Specifically the goals are:

1. To develop an RWV explant culture of avian (domestic chicken) liver and to determine if this can support the schizony and the hepatic life cycle of the avian malaria parasite *Plasmodium gallinaceum*.
2. To characterize the ability of the RWV Bioreactor to support the long term culture of three dimensional human liver explant tissue, and to assess the feasibility of using this RWV system to study the hepatic stage of *Plasmodium falciparum*.
3. To assess the ability of the RWV system to culture and maintain the normal morphology of mosquito midgut explants and to determine if the RWV bioreactor can support Oocyst development in the cultured intestinal wall of the insect.

BACKGROUND:

The World Health Organization has estimated that human malaria is responsible for over one million deaths worldwide per year. One long term goal of applied immunology has been to develop an effective vaccine against this parasite. This effort has been hampered to a large extent by the lack of an in vitro culture system which can

encompass the diverse multi-phyla developmental stages of the *Plasmodium* species. Of particular interest for immunological intervention, is the maturation of sporozoites into cryptozoites via a schizogony phase in the vertebrate liver. Unfortunately this stage is poorly characterized with respect to the expression of cell surface antigens with potential vaccine applications. It is possible that the RWV Bioreactor may be useful new technology to culture the cryptozoite stage of the *Plasmodium* sp. which in turn will assist the elucidation of such proteins.

Experiment Design: The initial stage of these experiments will focus on the ability of the RWV Bioreactor to support the three-dimensional culture of human and avian liver explants using only simple RPMI-1640 media with 10% Fetal Calf Serum. The maximum culture duration times will be determined with respect to morphology of the liver portal units and individual hepatocytes. The goal will be to maintain a recognizable three-dimensional cytoarchitecture for a minimum of 7 days RWV culture. The sporozoite to cryptozoite maturation time is between four to seven days depending on the *Plasmodium* species and we consider 7 days of RWV hepatocyte maintenance to be sufficient for these pilot experiments. When this system has been characterized, *Plasmodium gallinaceum* sporozoites will be added to fresh chicken RWV liver explants in an attempt to discern if this system can support sporozoite schizogony and maturation into the cryptozoite stage. Sporozoite maturation will be assessed by classical histology, outside consultations with the Armed Forces Institute of Pathology-Parasitic Disease Section, and immunocytochemistry. If successful, these experiments will be shifted to a protocol involving human liver explants and *Plasmodium falciparum* malaria with a focus on characterization of the surface proteins expressed during the cryptozoite stage of this human pathogen. Another aspect of *Plasmodium* sp. development of interest to infectious disease experts, is the Ookinete to sporozoite phase of the life cycle which takes place exclusively within the mosquito gut wall. The RWV Bioreactor will be assessed for its ability to culture mosquito midgut explants both before and after a blood meal, and to determine if this culture system can support ookinete to sporozoite maturation in vitro.

Preliminary Results:

1. Tissue explants of both avian (domestic chicken) and human liver have been maintained for a minimum of 7 days in the RWV bioreactor. Although areas of what appears to be apoptosis and a smaller degree of necrosis, are commonly observed around the central vein in some of the portal units, equal fields are observed that contain viable tissue with a normal three-dimensional cytoarchitecture. Bile is observed in the canaliculi of these areas indicating the functional preservation of the hepatocytes.
2. Histologically, the avian liver explants cultured in the RWV bioreactor appear to be able to support a small amount of *Plasmodium gallinaceum* cryptozoite development. We are in the process of confirming this histological result with immunohistochemistry.
3. The RWV bioreactor appears to be able to support the histological maintenance of *Aedes aegypti* midgut explants for a minimum of 5 days. In one experiment using a blood meal infected with *Plasmodium gallinaceum* trophozoites and gametocytes, morphology of the RWV cultured midgut suggested that ookinete development occurred in a few of the mosquito midgut explants. These experiments are in the process of being repeated.

Plans: Work will continue on refining and co-culturing *Plasmodium* sp. development stages with vertebrate tissue. A future experiment will focus on culturing cryptozoite infected liver explants with uninfected red blood cells in the RWV Bioreactor culture media to determine if the exoerythrocytic and erythrocytic pathways of the parasite's life cycle can take place in vitro. The eventual goal is to model as much of the organism's life cycle as possible and to use subtractive hybridization techniques to isolate developmental genes whose protein products might serve as a novel approach to vaccine development.

8. In Vitro production of Herpes Zoster Virus using human skin explants in the NASA Bioreactor.

Primary Investigators: Jeffery Cohen PhD, Department of Virology, National Institute for Allergy and Infectious Diseases.

Aims of Experiment: The apparent ability of the RWV bioreactor to provide a high-fidelity in vitro model for many human tissues, suggests this technology may have future applications for the rapid isolation and identification of new and as of yet uncharacterized viruses and bacteria associated with infectious human disease. To further explore the types of tissue and host/virus relations that can be successfully maintained in the RWV culture system, we will attempt the productive infection of RWV cultured human skin explants with the Herpes Zoster virus. This virus was chosen because of the difficulty in producing cell free virus in previous tissue culture systems, and the complexity of the stratified squamous epithelium which characterizes human skin.

BACKGROUND:

At this time, the pathogenesis of Herpes Zoster Virus (HZV) is poorly understood. Cell free virus isolates have proven to be extremely labile and it has proven difficult to study infection in single cell suspension tissue cultures. The virus initially attacks the epithelial covering of the epidermis to produce balloon degeneration of these cells with the formation of internuclear inclusions and multinucleate giant cells. It is uncertain at this time whether the initial site of attack occurs in the capillary endothelial cells or the basal epithelium of the skin. As infection progresses, the infected epidermis separates from the deeper dermis (acantholysis), and a clear vesicle develops roofed over by apparently uninfected stratum corneum. We hypothesize that the basal layer of the human skin is the site of initial infection and that the capillary endothelium is a second site of infection.

Experiment Design: We will attempt to culture full thickness human skin explants for long duration in the RWV bioreactor using simple RPMI-1640 media with Fetal Calf Serum (10%) and Timentin antibiotic. No exogenous growth factors will be added to the media. The skin samples will be obtained as a byproduct of normal surgical laparotomy or mastectomy. Skin samples from several ethnic groups will be utilized and particular attention will be given to the morphological preservation of both the basal cell layer of the skin, as well as the multi-layered squamous epithelial segment. Attention will also be directed towards the ability of the RWV Bioreactor to preserve histologically normal melanocytes. Samples of the RWV cultured tissue will be removed from the bioreactor at periodic intervals and assessed for normal morphology by standard histological techniques. These sections will also be prepared and subjected to immunohistochemistry to ensure that the cell surface markers which characterize normal human skin are maintained. Following this initial characterization, cell free HZV will be added to another series of human skin explants cultured in the RWV system. Periodic samples of the culture media and tissue will be taken and subjected to histology and plaque infectivity assay to determine if infection and free HZV virus production occurred within the system. Immunohistochemical methods and in-situ hybridization will then be used to determine the initial site of HZV infection in the explanted skin samples.

Preliminary Results:

1. Fragments of human skin can maintain normal histological morphology for a minimum of 2 weeks of RWV Bioreactor culture. This preservation includes an intact basal cell layer, histologically normal melanocytes, and normal appearing hair follicles.
2. Preliminary histology results suggest that explants of human skin cultured in the RWV Bioreactor can support the productive infection of the basal cell layer. This was evidenced by the characteristic balloon cell degeneration observed in the explants after infection with the HZV virus. Experiments are continuing using in situ hybridization and immunocytochemistry to document HZV infection of the basal cells.

3. Preliminary results of the plaque assays suggest that free HZV virus was released from the infected skin explants into the culture media after three days of infection. The experiments will be repeated using more sensitive ELISA techniques.

Plans: Initial pilot experiments have suggested that RWV explants of human skin can become productively infected with HZV virus. These experiments will be expanded using a more sensitive ELISA assay for the detection of free virus production into the culture media, and immunohistochemistry for the detection of viral specific proteins in paraffin embedded tissue sections. This work will be supported by in-situ hybridization studies on the this tissue sections. A time course series of infections will then be performed to assess if the capillary endothelium or the basal cell layer is infected first during the course of HZV pathogenesis. The ability of the RWV Bioreactor to culture a variety of different pathogenic organisms will be further assessed using this in vitro model of the skin. The human pathogen *Treponema pallidum* has so far been impossible to culture within the context of a three dimensional tissue micro-environment, and in spite of over 100 years of recognition, the mechanism for tissue destruction by this organism remains poorly characterized. Future experiments will focus on the ability of the RWV Bioreactor to support productive *T. pallidum* infection of human skin.

9. Use of the NASA bioreactor to improve the efficiency of vector transfer in gene therapy protocols.

Primary Investigators: Linda Maul PhD, National Center for Human Genome Research, NIH.

Aim of the Experiments: To employ the bioreactor to increase the efficiency of retroviral transfection of peripheral blood cells prior to human gene therapy. The RWV Bioreactor will be used in an attempt to increase the efficiency of retroviral vector transfer into co-cultured patient peripheral lymphocytes.

BACKGROUND:

An existing FDA protocol under consideration for human gene transfer therapy is dependent upon the LASN human fibroblast cell line which has been engineered to produce a delicate retroviral vector used to transfect human patient lymphocytes. Serious problems exist with respect to the low quantity of retrovirus production by the LASN cells and the low efficiency of retroviral transfection of the patient lymphocytes.

Experiment Design: The optimum conditions and media for RWV culture of the human LASN fibroblast cell line will be determined and the confluency of the culture for optimum retroviral vector production will be determined. Also, the maximum density and optimum amount of IL-2 will be determined for human peripheral mononuclear cells in the RWV Bioreactor. This data will be employed to co-culture the retroviral producing fibroblast cell line LASN together with peripheral mononuclear cells from a donor which are continuously activated and propagated in RWV medium containing IL-2. The efficiency of vector production and gene transfer will be assessed by existing ELISA and PCR techniques.

Preliminary Results:

1. Background data for the optimal conditions for LASN fibroblast and peripheral blood mononuclear cell culture have been established for the RWV Bioreactor. The optimum LASN culture conditions involve the use of microcarrier beads. Concentration of IL-2 and media replacement schedules have also been optimized.
2. To date, one experiment involving RWV co-culture of the LASN fibroblast line and microcarrier beads plus IL-2 activated human peripheral mononuclear cells has been performed. The results are in the process of analysis.

Plans: Experiments will continue in an effort to define the optimum conditions in the RWV Bioreactor for LASN and PBMC co-culture, and to determine the maximum amount of transfection efficiency that can be obtained in this system.

10. Protein crystal growth in the NASA Bioreactor.

Primary Investigators: Adrian Parsegian PhD, Laboratory of Structural Biology, Division of Computer Research and Technology, NIH.

Aim of Experiments : To assess the ability of the RWV Bioreactor to support protein crystal growth and to understand the forces that affect protein crystal structure and limitations in crystal size.

BACKGROUND:

The determination of tertiary protein structures by X-ray crystallography has lead to important new understandings with respect to protein structure and function. Unfortunately, X-ray crystallography is dependent upon the availability of large protein crystals which are difficult to form under conditions of normal earth gravity. The microgravity environment of space has proven unusually conducive to the formation of large protein crystal structures of many important biomolecules, but the cost of such space missions has limited the number of proteins which can be studied. Therefore there is an urgent need to understand the forces which limit protein crystal formation on earth. The RWV Bioreactor is capable of simulating many aspects of the microgravity environment and may be capable of providing important clues as to why protein crystals stop formation at a certain size.

Experiment Design: Protein crystal growth and formation will be studied using the RWV Bioreactor which will provide an isotropic environment capable of allowing crystal expansion in three-dimensions without the generation of disruptive shear forces. Protein saturated solutions will be subjected to long term RWV application and the formed crystals will be compared to those formed by conventional methods in order to evaluate whether their are differences in size, structure, and crystal symmetry.

Preliminary Data: Feasibility studies have now been completed which show that protein crystals can form and remain suspended in the bioreactor, and that these crystals can be observed visually during RWV operation.

Plans: A number of purified proteins will be subjected to crystallization in the RWV Bioreactor and these will be compared to the crystal structures formed by conventional techniques.

11. Long-term three-dimensional culture of intestinal tissue in the NASA Bioreactor to study the interactions of bacteria and parasites.

Primary Investigators: D. Hanes PhD, M. Miliotis PhD, and B. Tall PhD. Food and Drug Administration, Washington, D.C.

Aim of Experiments: To use the RWV Bioreactor to develop a high fidelity in vitro model of mammalian intestinal tissue and to study the interaction of enteric pathogens with this tissue and the mechanisms by which they cause disease. Attempts will also be made to use this RWV system to culture the *Cyclospora* sp. intestinal parasites.

BACKGROUND:

The tissue interactions and pathogenic mechanisms responsible for the majority of enteric infections of mammals, with the exception of select cases such as *Vibrio* sp., remain largely unknown. Much of the previous work in this field has involved growing cells on solid flat surfaces. These conditions by and large, do not promote cell differentiation and inhibits the comparison between in vitro models and the actual conditions in vivo. The RWV Bioreactor will be used to attempt to develop a high fidelity in vitro model of the mammalian epithelial gut wall which more closely approximates the conditions in vivo.

Experimental Design: CaCo-2 cells derived from human colon epithelial cells, will be seeded into the RWV Bioreactor and cultured for a period of 21 days. The cells will be sampled on three day intervals and fixed for later

electron microscopy to determine the ability of the bioreactor system to promote cell differentiation and the timing of this event. Upon the determination of proper RWV growth conditions, the system will be utilized for studies of bacterial infection and parasitic growth using standard microbiological and histological techniques and electron microscopy. Oocyst production will be studied in one species of amoebae.

Preliminary Results: Work is continuing on optimizing RWV Bioreactor culture conditions.

12. Long-term three-dimensional NASA Bioreactor culture of neonatal rat hypothalamus to study neurosecretory pathways.

Primary Investigators: Harold Gainer PhD, Division of Intramural Research, National Institute of Neurological Disorders and Stroke, NIH.

Aim of Experiments: To utilize RWV Bioreactor technology to culture neonatal rat hypothalamus in an effort to maintain the general cytoarchitecture and functionality of this tissue; in particular, the neurosecretory pathways.

BACKGROUND:

The most widely used technique for the culture of brain tissue explants has been the roller tube technique. Recently, a new method has been developed to allow long-term maintenance of brain explants using a millipore membrane with tissue at a gas/medium interface. The RWV Bioreactor has the potential to improve upon both these culture methods by allowing a better rate of mass transfer of nutrients and gases through the tissue under conditions of extremely low shear.

Experiment Design: Thin sections of neonatal rat hypothalamus will be obtained by standard procedures and cultured in the RWV Bioreactor using previously defined culture media. These cultures will be assessed with respect to the loss of glial or neuronal cell populations, the overgrowth of glial or astrocyte populations, and the loss or maintenance of neurosecretory function. The tissues will be assessed using standard histological techniques for the preservation of the native three-dimensional cytoarchitecture and the general hallmarks associated with each particular slice of the hypothalamus. Immunohistochemistry will be used to determine the presence and location of the oxytocin and vasopressin secreting cells.

Preliminary Results: Optimization of the RWV culture conditions is currently underway.

13. NASA Bioreactor epithelial cell studies on the unknown molecular pathogenesis of Mucopolipidosis Type 4 (ML4).

Primary Investigators: Ehud Goldin PhD, National Institute for Neurological Disorders and Stroke, NIH.

Aim of the Experiment: To develop a culture system which will enable molecular studies to be performed on cells from patients with Mucopolipidosis Type 4.

BACKGROUND:

ML4 is an autosomal recessive, developmental disorder of unknown cause. Clinically affected children develop motor retardation beginning in the first year of life and many cell types are found to contain abnormal storage bodies in the cytoplasm which contain an unknown material. The most common affected cell types are epithelial cells, typically from the cornea and stomach. There is no animal model for ML4 and the only tissue for research is from patients. To identify the primary etiology for this disease it is necessary to culture these epithelial cells, unfortunately this have proved impossible using conventional techniques for cell and tissue culture. This problem has significantly delayed the progress of our study.

Experiment Design: The RWV bioreactor will be utilized in an attempt to culture skin epithelial cells from primary skin biopsies taken from normal and ML4 patients, within the context of a normal three-dimensional tissue microenvironment. Three culture methods will be tried. (a) Skin epithelial cell suspensions will be prepared and an attempt will be made to form cellular aggregates in the RWV bioreactor. (b) Epithelial cell suspensions will be co-cultured in the RWV system using porous collagen microbeads. (c) Explants of human epidermis/dermis will be obtained as a byproduct of other elective surgeries and co-cultured with cell suspensions from ML4 patients in the RWV Bioreactor. It is hoped that the pre-existing microenvironment of the normal skin explants will prove conducive to ML4 epithelial cell attachment and long term proliferation.

Preliminary Results: Other bioreactor experiments have demonstrated the feasibility of culturing normal human skin explants in the RWV system. We are now awaiting the first ML4 tissue samples to begin experiments.

Plans: The RWV cultured ML4 epithelial cells will be used to provide study material for a wide range of immunohistochemistry and biochemical analysis of the ML4 cell components in an attempt to identify the precise biochemical pathway or pathways, involved in this disorder. This data may suggest methods for therapeutic intervention.

14. Differentiation of human dendritic cells in the NASA Bioreactor.

Primary Investigators: Peter Cohen PhD, Transplant Therapy Section, National Cancer Institute, and Charles Carter, Department of Transfusion Medicine, Clinical Center, NIH.

Aim of Experiments: To study the effects of a microgravity simulated environment on the differentiation and cell surface antigen expression of hematopoietic Dendritic Cells (DC) using the RWV Bioreactor.

BACKGROUND:

Human dendritic cells are responsive to circulating antigen only at specific times of their maturation/differentiation life cycle and the individual characteristics of these dendritic cell stages have been shown to be independently regulated at the molecular level by a variety of factors which include surface contact and intercellular calcium mobilization. The dendritic cell differentiation pattern is encompassed by the expression of CD83 (an activation marker), the *de novo* expression of B7.1 and the down regulation of the CD 14 lipopolysaccharide receptor. The RWV Bioreactor provides the opportunity to culture dendritic cells without the surface contact stimulation provided by other culture methods.

Experiment Design: The pilot experiment will subject freshly isolated human hematopoietic dendritic cells to RWV Bioreactor culture using defined media. The expression of CD 83, B7.1 antigen and CD 14 will be assessed by immunocytochemistry and FACS analysis. The maturation / differentiation cycle of these cells will then be assessed in the simulated microgravity environment of the RWV system to determine any change in the expression of these markers.

Preliminary Results:

1. In the initial pilot experiment, isolated hematopoietic dendritic cells were shown to exhibit a different modulation of the CD 14 cell surface antigen when compared to cells grown under standard culture conditions.

Plans: These experiments will continue and the nature of the different CD14 expression pattern in the RWV cultured cells will be investigated on the molecular level. The ability to differentially regulate individual dendritic cell characteristics via culturing the cells in a simulated microgravity environment may be useful in preparing dendritic cells for particular clinical uses such as vaccine strategies.

15. Use of the role of gap junctions in NASA Bioreactor to evaluate lymphoid tissue function.

Primary Investigators: Andrew Harris PhD, John Hopkins University.

Aim of Experiments: The cellular interactions involved in the proper function of the immune system are complex and depend upon the integrity of the normal tissue cytoarchitecture. There is increasing evidence that normal immune tissue function involves the specific regulation of gap junction mediated interactions. The purpose of this project is to explore the role of the intercellular communication mediated by gap junctions in the response of lymphoid tissue to antigen (antibody production) and infection (e.g., by HIV). This work builds upon the results recently obtained from other ongoing projects at the NASA/NIH Center for Tissue Culture.

Specifically our goals are:

1. To establish that the occurrence of gap junction communication in RWV cultured lymphoid tissue, correlates with that inferred from in situ and in vivo studies.
2. To determine the effects of experimental modulation of gap junction communication on the ability of RWV cultured lymphoid tissue to mount an immune response.
3. To explore the changes in gap junction communication in RWV cultured lymphoid tissue that occurs during HIV infection, with the aim of elucidating a mechanism for the compromised immune function that characterizes HIV disease.

BACKGROUND:

Gap junctions are intercellular channels which mediate the intercellular diffusion of ions and small signaling molecules up to 14 Angstroms in diameter. This size range includes most of the known cytoplasmic signaling molecules such as calcium, cyclic nucleotides and the inositol triphosphates. The chemical signaling through such channels appears to be important for normal development and differentiated tissue function. The disruption of normal gap junctions has severe consequences and structural abnormalities in the gap junction associated proteins lead to severe developmental defects in mice and genetic diseases in humans. The human immune system involves a complex network of cellular interactions and morphological gap junctions between various immune cells have been described for many years. The functional expression of the Connexin group of gap junction proteins has recently been shown to correlate with changes in immune system function.

Experiment Design: Using techniques previously developed by the NASA/NIH Center, we will determine the identity and distribution of the connexins in freshly obtained and cultured human lymphoid tissue. This data will be used to assess if this RWV cultured tissue retains a normal pattern of connexin expression. RWV cultures will be challenged with tetanus toxoid and the changes in connexin expression determined by immunohistochemical and biochemical techniques. Gap junction function will then be modulated during tetanus toxoid challenge and the culture viability and antibody production determined. Agents which decrease or eliminate gap junction communication will be added to the RWV cultured lymphoid tissue to determine whether gap junctions are necessary for the maintenance of functional lymphoid tissue. Similar studies will be performed using HIV infected cultures. The patterns of communication within the cultures will be determined by the injection of fluorescent tracers into cells under confocal microscopy. This will provide structural and physiological data on the nature of the changes in intercellular communication under the various conditions.

Preliminary Results:

1. Initial experiments are currently underway using an antibody specific for Cx43 to immunostain fresh human tonsillar tissue.

2. Initial cultures have been set up with glycyrrhetic acid in the culture media to block gap junctional activity and to assess the morphology of the cultured lymphoid tissue.

Plans: The system will continue to be developed according to the above outlined scheme. The immediate priority is to obtain reliable immunohistochemical staining of fresh tissue and RWV cultured explants and to continue RWV culture experiments in the presence of modulator compounds.

III. Microgravity Science & Applications Bibliographic Citations for FY 1996

- **Flight Research Tasks**
 - Biotechnology III-1057
 - Combustion Science III-1058
 - Fluid Physics III-1063
 - Fundamental Physics..... III-1067
 - Materials Science III-1069
- **Ground Research Tasks**
 - Biotechnology III-1079
 - Combustion Science III-1092
 - Fluid Physics III-1099
 - Fundamental Physics..... III-1120
 - Materials Science III-1123
- **ATD**
 - Advanced Technology Development III-1137
- **Technology Transfer** III-1139

How to Order Publications Cited in this Document:

Copies of many of the documents cited in the bibliography published here are available from the **Center for AeroSpace Information (CASI)**, a NASA Scientific and Technical Information (STI) program facility. Prices are determined by the number of pages of each document and whether paper or microfiche copy material is ordered.

NASA Center for AeroSpace Information (CASI)
P.O. Box 8757
Baltimore, MD 21240-0757
Telephone: 301 621-0390, FAX: 301 621-0134

Flight: Biotechnology

Ban, N., and McPherson, A. The structure of satellite panicum mosaic virus at 1.9 Å resolution. *Nature Structural Biology*, vol. 2, no. 10, 882-890 (1995).

Ban, N., Day, J., Wang, X., Ferrone, S., and McPherson, A. Crystal structure of an anti-anti-idiotypic shows it to be self-complementary. *J. Mol. Biol.*, vol. 255, 617-627 (1996).

Ban, N., Larson, S.B., and McPherson, A. Structural comparison of the plant satellite viruses. *Virology*, vol. 214, 571-583 (1995).

Bray, T.L., Powell, D.L., Kim, L.J., Gray, R.J., Le, T., Askew, R.P., Harrington, M.D., Rosenblum, W.M., Wilson, W.W., and DeLucas, L.J. New Crystallization Systems Envisioned for Microgravity Studies. *J. Appl. Crystall.*, (1996, in revision).

Canady, M.A., Larson, S.B., Day, J., and McPherson, A. Crystal structure of turnip yellow mosaic virus. *Nat. Struc. Biol.*, vol. 3, no. 9, 771-781 (1996).

Carter, D.C. "PCAM and DCAM, Summary of Flight Results 1994-96." Protein Crystal Growth Workshop, Panama City Beach, Florida, May 1996.

Carter, D.C. "PCAM and DCAM, Summary of Flight Results 1995-96." Gordon Research Conference, New Hampshire, June 1996.

Carter, D.C. "PCAM and DCAM Hardware and Facility." International Microgravity Protein Crystal Growth Workshop, University of California, Riverside, 1996.

Cole, T., Kathman, A., Koszelak, S., and McPherson, A. Determination of the local refractive index for protein and virus crystals in solution by Mach-Zehnder interferometry. *Anal. Biochemistry*, vol. 231, 92-98 (1995).

Giegé, R., Drenth, J., Ducruix, A., Saenger, W., and McPherson, A. Crystallogensis of biological macromolecules. Biological, microgravity, and other physico-chemical aspects. *Prog. Crystal Growth and Charact.*, vol. 30, 237-281 (1995).

Gorti, S., Zuk, W.M., Ward, K.B., Tanaka, T., and Yang, H. "Lysozyme Diffusion in the Vicinity of Crystal Surfaces."

Harris, L.J., Skaletsky, E., and McPherson, A. Crystallization of intact Monoclonal antibodies. *Proteins*, vol. 23, 285-289 (1995).

Jessup, J.M., Goodwin, T.J., Garcia, R., and Pellis N.R. "STS-70: First Flight of EDU-1." Society for In Vitro Biology, San Francisco, CA, June 1996.

Ko, T.-P., Williams, R., and McPherson, A. The crystal structure of a ribonuclease B + d(pA)₄ complex. *Acta Cryst.*, vol. D52, 160-164 (1996).

Land, T.A., Malkin, A.J., Kuznetsov, Yu.G., McPherson, A., and DeYoreo, J.J. Mechanisms of protein crystal growth: An atomic force microscopy study of Canavalin crystallization. *Phys. Rev. Letters*, vol. 75, no. 13, 2774-2777 (1995).

Malkin, A.J., Kuznetsov, Y.G., Glantz, W., and McPherson, A. Atomic force microscopy studies of surface morphology and growth kinetics in thaumatin crystallization. *J. Phys. Chem.*, vol. 100, 11736-11743 (1996).

Malkin, A.J., Kuznetsov, Yu.G., and McPherson, A. Incorporation of microcrystals by growing protein and virus crystals. *Proteins*, vol. 24, 247-252 (1996).

Malkin, A.J., Land, T.A., Kuznetsov, Yu.G., McPherson, A., and DeYoreo, J.J. Investigation of virus crystal growth by in situ atomic force microscopy. *Phys. Rev. Letters*, vol. 75, no. 13, 2778-2781 (1995).

Malkin, A.J., Kuznetsov, Yu.G., Land, T.A., DeYoreo, J.J., and McPherson, A. Mechanisms of growth for protein and virus crystals. *Nature Structural Biology*, vol. 2, no. 11, 956-959 (1995).

McPherson, A. "Nature and Effects of Impurities in Macromolecular Crystals." ICCBM Conference, Hiroshima University, Hiroshima City, Japan, November 12-17, 1995.

McPherson, A. "Macromolecular Crystal Growth in Microgravity." 6th International Space Conference of Pacific Basin Societies, Los Angeles, California, December 6-8, 1995.

McPherson, A. "Macromolecular Crystal Growth in Microgravity." 1st Conference on Commercial Development of Space - Space Technology & Applications Forum (STAIF 96), Albuquerque, New Mexico, January 7-11, 1996.

McPherson, A. "Presentation of Research and Hardware Development Plans FOR ISS-PCG (NASA MSFC)." International Workshop on Microgravity Biotechnology for the International Space Station (ISS), University of California - Riverside Campus, February 15-16, 1996.

McPherson, A. "Defect Structure and Density in Macromolecular Crystals." Protein Crystal Growth Conference, Panama Beach City, Florida, April 28-30, 1996.

McPherson, A. "The Nucleation Phase in Macromolecular Crystallization." International Meeting on Recent Advances in Macromolecular Crystallization, Bischenberg, France, June 2-4, 1996.

McPherson, A. "Macromolecular Crystal Growth in Microgravity." World Congress on In Vitro Biology, San Francisco, California, June 22-27, 1996.

McPherson, A. "Macromolecular Crystallization." IUCr XVII Congress and General Assembly, Seattle, Washington, August 8-17, 1996.

Zuk, W.M., Gorti, S., and Ward, K.B. "Investigation of Protein Crystal Growth Mechanisms in Microgravity." Annual Protein Crystal Growth Conference, Panama City, Florida, April 28-30, 1996.

Flight: Combustion Science

Abid, M. and Ronney, P.D., "Buoyancy effects on propagating chemical fronts in aqueous solution." 48th Annual Meeting, Division of Fluid Dynamics, American Physical Society, Irvine, CA, November 19-21, 1995.

Anthenien, R.A., Walther, D.C., and Fernandez-Pello, A.C., "An experimental study of smolder ignition of polyurethane foam." Western States Section/The Combustion Institute, 1995 Fall Meeting, Stanford University, Stanford, CA, October 31, 1995.

Bahadori, M.Y., "Laminar, transitional, and turbulent jet diffusion flames in microgravity." Center for Energy and Combustion Science, University of California, San Diego, October 1996.

Bahadori, M.Y., Small, J.F., Hegde, U., and Stocker, D.P., "Single-point measurements and predictions of radiative loss from buoyant and non-buoyant jet diffusion flames." Proceedings of the Central States Meeting of The Combustion Institute, St. Louis, MO, May 1996.

Bahadori, M.Y., Small, J.F., Hegde, U., and Stocker, D.P., "Measurements and predictions of the temperature field of a microgravity diffusion flame." Proceedings of the Western States Meeting of The Combustion Institute, Los Angeles, CA, October 1996.

Bahadori, M.Y., Zhou, L., Stocker, D.P., and Hegde, U., "Measurements of flame flicker under different gravitational levels." Proceedings of the Fall Eastern States Meeting of The Combustion Institute, Hilton Head, SC, 1996.

Bhattacharjee, S., Altenkirch, R.A., and Sacksteder, K.R., "The effect of ambient pressure on flame spread over thin cellulosic fuel in a quiescent, microgravity environment." J. Heat Transfer, vol. 118, pp.181-190 (1996).

Bhattacharjee, S., West, J., Altenkirch, R.A., "Determination of the spread rate in opposed-flow flame spread over thick solid fuels in the thermal regime." presented at the 26th International Symposium on Combustion, Naples Italy, 1996.

Bhattacharjee, S., West, J. and Altenkirch, R.A., "Determination of the spread rate in opposed-flow flame spread over thick solid fuels in the thermal regime." Twenty-Sixth International Symposium on Combustion, The Combustion Institute, August, 1996.

- Choi, M.Y. and Lee, K-O., "Investigation of sooting in microgravity droplet combustion." Proceedings of the Central States Section Meeting of the Combustion Institute, St. Louis, MO, May, 1996.
- Choi, M.Y. and Lee, K-O., "Investigation of sooting in microgravity droplet combustion." 26th Symposium (International) on Combustion, The Combustion Institute, 1996.
- Delichatsios, M., "Creeping flame spread: energy balance and applications to practical materials." presented at the 26th International Symposium on Combustion, Naples Italy, 1996.
- Dietrich, D.L., Haggard, J.B. Jr., Dryer, F.L., Nayagam, V., Shaw, B.D., and Williams, F.A. "Droplet combustion experiments in Spacelab." Twenty Sixth International Symposium, Naples, Italy, July 22-August 2, 1996.
- Faeth, G.M., "Laminar Soot Process (LSP) experiment." MSL-1: Third IWG Meeting, Marshall Space Flight Center, Huntsville, March 1996.
- Faeth, G.M. and Koylu, U.O., Soot morphology and optical properties in nonpremixed turbulent flame environments. Combust. Sci. Tech., vol. 108, no. 4-6, pp. 207-229 (October, 1995).
- Faeth, G.M., and Koylu, U.O., "Structure and optical properties of flame-generated soot." Proceedings of the 8th International Symposium on Transport Phenomena in Combustion, Taylor and Francis New York, September 1996.
- Fendell, F.E. and Mitchell, J.A., Feasibility of planar, unidirectional-flow diffusion flames in earth gravity. Comb. Sci. & Tech., (October, 1995).
- Fendell, F.E. and Wu, F., Unsteady planar diffusion flames: ignition, travel, burnout. Comb. Sci. & Tech., vol. 107, pp. 93-126 (October, 1995).
- Fendell, F.E. and Wu, F., Diffusion-flame burning of fuel-vapor pockets in oxidizer for general Lewis numbers. Combustion and Flame, vol. 105, pp. 1-14 (1996).
- Hegde, U., et al., "Microgravity environment and its effects on science." Proceedings of the AIAA-96-0401, Invited Panel Presentation at the AIAA 34th Aerospace Sciences Meeting, Reno, NV, January 1996.
- Hegde, U., Stocker, D.P., and Bahadori, M.Y., "Temperature correlations in a pulsed microgravity diffusion flame." Proceedings of the AIAA-96-0261, AIAA 34th Aerospace Sciences Meeting, Reno, NV, January 1996.
- Hegde, U., Stocker, D.P., and Bahadori, M.Y., "Unsteady diffusion flames in microgravity." Proceedings of the Fall Eastern States Meeting of The Combustion Institute, Hilton Head, SC, 1996.
- Hegde, U., Zhou, L., and Bahadori, M.Y., Winner of the SAIC 1995 Publications Prize in Physics: "The transition to turbulence of microgravity gas jet diffusion flames". Combustion Science and Technology, vol. 102, no. 1-6, pp. 95, 1994 (November 1996).
- Held, T.J., Marchese, A.J., and Dryer, F.L., A semi-empirical reaction mechanism for -n-heptane oxidation and pyrolysis. Combustion Science and Technology, (April, 1996).
- Jiang, C-B, T'ien, J.S., "Upward flame spread over a thin solid in reduced gravity: model calculations with flame radiation." presented at the 46th International Astronautical Federation Congress, Oslo Norway, October 1995.
- Jiang, C-B, T'ien, J.S., and Shih, H-Y, "Model calculation of steady upward flame spread over a thin solid in reduced gravity." Twenty-Sixth Symposium (International) on Combustion, Naples Italy, July 1996.
- Jiang, C-B, T'ien, J.S., and Shih, H-Y, "A numerical study of flame radiation effect of forced concurrent-flow flame spread over a solid using discrete ordinates method." presented to the Sixth International Conference on Numerical Combustion, New Orleans, March 1996.
- Jiang, Ching-Biau, T'ien, J.S. and Shih, Hsin-Yi "Model calculation of steady upward flame spread over a thin solid in reduced gravity." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28-August 2, 1996.

Kashiwagi, T., Mcgrattan, K.B., Olson, S.L., Fujita, O., Kikuchi, M., and Ito, K. "Effects of slow wind on localized radiative ignition and transition to flame spread in microgravity." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28-August 2, 1996.

Koylu, U.O. and Faeth, G.M., "Spectral extinction coefficients of soot aggregates from turbulent diffusion flames." Proceedings of the Fall Technical Meeting, Eastern Section of the Combustion Institute, Pittsburgh, PA, pp. 211-214, October 1995.

Koylu, U.O. and Faeth, G.M., Spectral extinction coefficients of soot aggregates from turbulent diffusion flames. J. Heat Trans, vol. 118, no. 2, pp. 415-421 (1996).

Koylu, U.O. and Faeth, G.M., Spectral extinction coefficients of soot aggregates from turbulent diffusion flames. J. Heat Trans, vol. 118, no. 2, pp. 415-421 (1996).

Lee, C.J., Tomboulides, A.G., Orszag, S.A., Yetter, R.A., and Dryer, F.L., "A transient two-dimensional chemically reactive flow model: Fuel particle combustion in a non-quiescent environment." Twenty Sixth International Symposium, Naples, Italy, July 22-August 2, 1996.

Lee, J.C., "Simulations of two dimensional chemically reactive flow." Ph.D. Thesis, Mechanical and Aerospace Engineering Dept., Princeton University, Princeton, NJ, MAE Report No. 2063-T, June, 1996.

Lee, J.C., Tomboulides, A.G., Orszag, S.A., Yetter, R.A., and Dryer, F.L. Integrated asymptotic analysis and numerical simulation of laminar flow reactors. Combustion Science and Technology, (July 17, 1996).

Lee, J.C., Tomboulides, A.G., Orszag, S.A., Yetter, R.A., and Dryer, F.L., "Asymptotic and numerical modeling of laminar flow reactors." Third Workshop on Modeling of Chemical Reaction Systems, Heidelberg, Germany, July 24-26, 1996.

Lee, J.C., Tomboulides, A.G., Orszag, S.A., Yetter, R.A., and Dryer, F.L., "Asymptotic and numerical modeling of laminar flow reactors." Poster presentation, Twenty-Sixth International Symposium on Combustion, Poster No. 04-84, Naples, Italy, July 22-August 2, 1996.

Lee, J.C., Yetter, R.A., and Dryer, F. L., Numerical simulation of laser ignition of an isolated carbon particle in quiescent environment. Combustion and Flame, 105, 591 (1996).

Lee, K.-O., Jensen, K.A., and Choi, M.Y., "Investigation of sooting in normal-gravity droplet combustion using light extinction and gravimetric techniques." Twenty-Sixth International Symposium on Combustion, The Combustion Institute, 1996.

Lee, Kyeong-Ook, Jensen, K.A., Choi, M.Y. "Measurement of soot volume fraction of single droplets using light extinction technique." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28-August 2, 1996.

Lin, K.-C., "Soot control in laminar opposed-jet diffusion flames." Fluid and Gas Dynamics Seminar, Department of Aerospace Engineering, The University of Michigan, October 1995.

Lin, K.-C. and Faeth, G.M., "Effects of hydrodynamics on soot formation in hydrocarbon-fueled laminar opposed jet diffusion flames." Proceedings of the Fall Technical Meeting, Eastern Section of the Combustion Institute, Pittsburgh, P.A. pp.423-426, October 1995.

Lin, K.-C. and Faeth, G.M., "Structure of laminar permanently-blue opposed-jet hydrocarbon fueled diffusion flames." Proceedings of Spring Technical Meeting, Central States Section, The Combustion Institute, Pittsburgh, pp. 110-115, May 1996.

Lin, K.-C. and Faeth, G.M., Effects of hydrodynamics on soot formation in laminar opposed-jet diffusion flames. J. Prop. Power, vol. 12, no. 4, pp. 691-698 (1996).

Lin, K.-C., Sunderland, P.B., and Faeth, G.M., Soot nucleation and growth in acetylene/air laminar coflowing jet diffusion flames. Combust. Flame, vol. 104, no. 3, pp. 369-375 (1996).

- Marchese, A.J., "Combustion of single and bicomponent liquid droplets: Detailed kinetic modeling and microgravity experiments." PhD. Thesis, Mechanical and Aerospace Engineering Dept., Princeton University, Princeton, JN, MAE Report No. 2081-T, 1996.
- Marchese, A.J., and Dryer, F.L., Effect of liquid mass transport on the combustion and extinction of Bi component liquid droplets of methanol and water. *Combustion and Flame*, 105, 104 (1996).
- Marchese A.J., and Dryer, F.L., The effect of non-luminous thermal radiation in microgravity droplet combustion. *Combustion Science and Technology*, (July 18, 1996).
- Marchese, A.J., and Dryer, F.L., The effect of non-luminous thermal radiation in microgravity droplet combustion. *Mechanical and Aerospace Engineering*, 2074, (1996).
- Marchese, A.J. and Dryer, F.L., "The effect of non-luminous gas phase radiation on the combustion of large droplets in microgravity." Twenty-Sixth International Symposium on Combustion, Naples, Italy, Poster No. 5-083, July 22-August 2, 1996.
- Marchese, A.J., Dryer, F.L., Nayagam, V., "Microgravity combustion of methanol and methanol/water droplets: Drop tower experiments and model predictions." Twenty Sixth International Symposium, Naples, Italy, July 28-August 2, 1996.
- Marchese, A.J., Dryer, F.L., Nayagam, V., and Colantonio, R., "Hydroxyl radical chemiluminescence imaging and the structure of microgravity droplet flames." Twenty Sixth International Symposium, Naples, Italy, July 28-August 2, 1996.
- McGrattan, K.B., Kashiwagi, T., Baum, H.R., and Olson, S.L., Effects of ignition and wind on the transition of flame spread in a microgravity environment. *Combustion and Flame*, (October, 1995).
- Miller, F.J., Vickerman, M., and Ross, H.D. Video-based, colorized particle image flow visualization. *NASA Tech Brief*, (1996).
- Pearlman, H., Excitability in high-lewis number premixed gas combustion. *Combustion and Flame*, (1996).
- Pearlman, H., "Spiral wave and target patterns on the surface of a freely-propagating premixed gas flame." Dynamics Day Workshop, Houston, TX, January 3-6, 1996.
- Pearlman, H., "Excitability in high-lewis number premixed gas combustion." West Virginia University Department of Chemistry, August 8, 1996.
- Pearlman, H., "Excitability in High-Lewis number premixed gas combustion." West Virginia University Department of Chemistry, August 8, 1996.
- Pearlman, H. "An excitable premixed gas reaction." Department of Chemistry, West Virginia University, Morgantown, WV, August 8, 1996.
- Pearlman, H. Excitability in high-Lewis number premixed gas combustion. *Combustion and Flame Paper No. 1612*, (accepted April, 1996).
- Pearlman, H., Stocker, D., Gotti, D., Urban, D., Ross, H., and Sours, T. Demonstrating reduced gravity. *The Physics Teacher*, vol. 34, No. 3, 172-176 (1996).
- Ronney, P.D., "Combustion at zero gravity." 36th Israel Annual Conference on Aerospace Sciences, Haifa, Israel, February 21-22, 1996.
- Ronney, P.D., "Dynamics and pattern formation in propagating chemical fronts in buoyant and turbulent flows." 15th Dynamic Days, Houston, Texas, January 3-6, 1996.
- Ronney, P.D., "Combustion experiments on spacelab mission MSL-1." 6th International Space Conference of Pacific Basin Societies, Marina del Rey, CA, December 6-8, 1995.

Ronney, P.D., "Dynamics and pattern formation in propagating chemical fronts in buoyant and turbulent flows ." 15th Dynamics Days Texas, Houston, TX, January 3-6, 1996.

Ronney, P.D., "Dynamics and pattern formation in propagating chemical fronts in buoyant and turbulent flows." California Institute of Technology, May 17, 1996.

Ronney, P.D. and Abid, M., "Buoyancy effects on propagating chemical fronts in aqueous solution." 48th Annual Meeting, Division of Fluid Dynamics, American Physical Society, Irvine, CA, November 21-22, 1995.

Ronney, P.D., and Wu, M.-S., "Numerical simulation of flame ball structure and stability." 6th SIAM Conference on Numerical Combustion, New Orleans, LA, March 4-6, 1996.

Ronney, P.D. and Wu, M.-S., "Numerical simulation of flame ball structure and stability ." 6th SIAM Conference on Numerical Combustion, New Orleans, March 4-6, 1996.

Ronney, P.D. and Zhu, J.-Y., "Numerical simulation of buoyant chemical front propagation in Hele-Shaw flow." 6th SIAM Conference on Numerical Combustion, New Orleans, LA, March 4-6, 1996.

Ronney, P.D. and Zhu, J.-Y., "Numerical simulation of buoyant chemical front propagation in Hele-Shaw flow." 6th SIAM Conference on Numerical Combustion, New Orleans, March 4-6, 1996.

Ross, H.D. and Miller, F.J. "Detailed experiments of flame spread across deep butanol pools." 26th International Symposium on Combustion, The Combustion Institute, Naples, Italy, 1996.

Schiller, D.N. and Sirignano, W.A. "Opposed-flow flame spread across n-propanol pools." 26th International Symposium on Combustion, the Combustion Institute, Naples, Italy, 1996.

Schiller, D.N. and Sirignano, W.A. "Opposed-flow flame spread across n-butanol." 34th AIAA Aerospace Sciences Meeting, Reno, NV, 1996, Paper No. 96-0216.

Schiller, D.N., Ross, H.D. and Sirignano, W.A. Computational Analysis of flame spread across alcohol pools. Comb. Sci. Tech., (1996).

Shultz, D.A., Matkowsky, B.J., Volpert V.A., and Fernandez-Pello, A.C., Forced forward smolder combustion. Combustion and Flame , (1996).

Shy, S. S., Jang, R. H., and Ronney, P.D., Laboratory simulation of flamelet and distributed models for premixed turbulent combustion using aqueous autocatalytic reactions. Combustion Science and Technology, vol. 113-114, 329-340 (1996).

Sirignano, W.A. and Schiller, D.N. "Mechanisms of Flame Spread Across Condensed-Phase Fuels," to appear in "Physical and Chemical Aspects of Combustion: A Tribute to Irvin Glassman." Edited by: Sawyer, R.F. and Dryer, F.L. Gordon and Breach Publishers, Inc., 1996.

Stocker, D.P., Olson, S.L., Urban, D., Torero, J.L., Walther, D., and Fernandez-Pello, A.C. "Small scale smoldering combustion experiments in microgravity." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28-August 2, 1996.

T'ien, J.S., Sacksteder, K.R., and Ferkul, P.V., Solid inflammability boundary at low speed. Science Requirements Document, (June 1996).

Torero, J.L., and Fernandez-Pello, A.C., Forward smolder of polyurethane foam in a forced air flow. Combustion and Flame, (1996).

Tse, S., Anthenien, R., Miyasaka K., and Fernandez-Pello, A.C., "A novel technique for ultrasonic imaging of smoldering combustion." 26th International Symposium on Combustion, August 2, 1996.

Tse, S.D., Fernandez-Pello, A.C., and Miyasaka, K., "Controlling mechanisms in the transition from smoldering to flaming of flexible polyurethane foam." 26th International Symposium on Combustion, (in press 1996).

- Walter, D., Urban, D., and Fernandez-Pello, A.C., "Smoldering combustion experiments in microgravity." 26th International Symposium on Combustion, August 2, 1996.
- West, Tang, Altenkirch, R.A., Bhattacharjee, S., Sacksteder, K., and Delichatsios, M., "Quiescent flame spread over thick fuels in microgravity." presented at the 26th International Symposium on Combustion, Naples Italy, 1996.
- Wu, M.S., Ronney, P.D., Colantonio, R.O., VanZandt, D.M., "Detailed numerical simulation of flame ball structure and dynamics." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28-August 2, 1996.
- Xu, F., "Soot nucleation and growth in laminar premixed flames." Fluid and Gas Dynamics Seminar, Department of Aerospace Engineering, The University of Michigan, November 1995.
- Xu, F., Sunderland, P.B. and Faeth, G.M., Soot formation in laminar premixed ethylene/air flames at atmospheric pressure. Combustion and Flame, (In press 1996).
- Xu, F., Sunderland, P.B., and Faeth, G.M. "Measurements and predictions of soot formation in laminar premixed flames." Proceedings of Spring Technical Meeting, Central States Section, The Combustion Institute, Pittsburgh, May 1996.
- Zhang, B.L. and Williams, F.A., "Theoretical studies of methanol droplet combustion based on results from the Shuttle spacelab during the USML-2 mission." 47th International Astronautical Congress, IAF-96-J.3.12, Beijing, 1996.
- Zhang, B.L. and Williams, F.A., "Simplified analyses of methanol droplet combustion for comparison with microgravity experimental results." 34th Aerospace Sciences Meeting and Exhibit, AIAA-96-0263, Reno, 1996.
- Zhang, B.L., and Williams, F.A., "Alcohol droplet combustion." 46th International Astronautical Congress, IAF-95-J.1.05, Oslo, Norway, 1995; Acta Astronautica, in press, 1996.

Flight: Fluid Physics

- Balasubramaniam, R. and Subramanian, R.S. Thermocapillary bubble migration - Thermal boundary layers for large Marangoni numbers. Int. J. Multiphase Flow, vol. 22, no. 3, 593-612 (1996).
- Balasubramaniam, R., Lacy, C.E., Wozniak, G., and Subramanian, R.S. Thermocapillary migration of bubbles and drops at moderate values of the Marangoni number in reduced gravity. Physics of Fluids, vol. 8, no. 4, 872-880 (1996).
- Campbell, T. and Koster, J.N. Modeling on convection in Gallium encapsulated by silicone oils. Acta Astronautica, vol. 35, 805-812 (1995).
- Chaikin, P.M., Zhu, J., Russel, W.B., "Dynamics of disorder-order transitions in hard sphere colloidal dispersions in microgravity." Proceedings of Third Microgravity Fluid Physics Conference, 1996.
- Chen, Q., Rame, E., and Garoff, S., Experimental studies on the parametrization of liquid spreading and dynamic contact angles. Colloids and Surfaces, (1996).
- Chen, Q., Rame, E., and Garoff, S., The velocity field near moving contact lines. J. of Fluid Mech., (1996).
- Costes, N.C., and Sture, S. "Issues on geomechanics." Proceedings of the ASCE 5th International Conference on Space '96, pp 516-520, Albuquerque, New Mexico, 1996.
- Durian, D.J. "The melting of aqueous foams." Third Microgravity Fluid Physics Conference, NASA Lewis Research Center, Cleveland, OH, 1996.
- Durian, D.J., Gopal, A.D., Vera, M.U., and Langer, S.A. "The melting of aqueous foams." NASA Conference Publication (1996).
- Ferrell, R.A., "A brief survey of the equilibrium and transport properties of critical fluids and the degree to which microgravity is required for their experimental investigation." Proceedings of the Third Microgravity Fluid Physics Conference, Cleveland OH, NASA Conference Publication 3338, pp. 53-57, June, 1996.

- Ferrell, R.A., "Modulated order parameter." Max-Planck-Institut fuer Physik Komplexer Systeme, Dresden Germany, June, 1996.
- Gang, H., Krall, A.H., and Weitz, D.A., Thermal fluctuations of the shapes of droplets in dense and compressed emulsions. *Phys. Rev. E*, 52, 6289-6302 (1995).
- Hart, J.E., and Kittelman, S. Instabilities of the sidewall boundary layer in a differentially driven rotating cylinder. *Physics of Fluids*, vol. 8, 692-696 (1996).
- Hart, J.E., and Mundt, M.D. Instability of oscillatory Stokes-Stewartson layers. *J. Fluid Mech.*, vol. 311, 119-140 (1996).
- Hmelo, A.B., Battaile, C.C., and Wang, T.G. The velocity of sound in liquid succinonitrile near the melting temperature. *Journal of Acoustical Society of American*, (in press).
- Jacobs, J.W. and Niederhaus, C.E., "An experimental study of Richtmyer-Meshkov instability." NASA 3rd Fluids Physics Conference, NASA Lewis Research Center, June 13-15, 1996.
- Jenkins, J.T., "Inelastic behavior of random arrays of identical spheres." UTAM Symposium on the Mechanics of Granular and Porous Materials. (N.A. Fleck and A. Cocks, Eds.) Kulwer, Sandia Labs, 1996.
- Jenkins, J.T. and Hanes, D.M. A sheared sheet of colliding grains driven from above by a turbulent flow. *J. of Fluid Mechanics*, (in press).
- Jenkins, J.T. and Louge, M.Y., "Microgravity Segregation in Binary Mixtures of Inelastic Spheres Driven by Velocity Fluctuation Gradients." *Proceedings of the Third Microgravity Fluid Physics Conference*, NASA, 1996.
- Jenkins, J.T. and Louge, M.Y. On the flux of fluctuation energy through a flat, frictional wall bounding rapid flows of inelastic frictional spheres. *Physics of Fluids*, (1996).
- Kamotani, Y., Chang, A., and Ostrach, S., Effects of heating mode on steady axisymmetric thermocapillary flows in microgravity. *Journal of Heat Transfer*, vol. 118, pp. 191-197 (1996).
- Kamotani, Y., Masud, J., and Pline, A., Oscillatory convection due to combined buoyancy and thermocapillarity. *Journal of Thermophysics and Heat Transfer*, vol. 10, pp. 102-108 (1996).
- Kamotani, Y., Ostrach, S., and Pline, A., A thermocapillary convection experiment in microgravity. *Journal of Heat Transfer*, vol. 117, (November 3, 1995).
- Kamotani, Y., Ostrach, S., and Pline, A., "Some temperature field results from the thermocapillary flow experiment aboard USML-2 spacelab." presented at the 31st Scientific Assembly of COSPAR, Birmingham, England, July 14-21, 1996.
- Kang, S.Y., Sangani, A.S., Tsao, H.K., and Koch, D.L. Rheology of dense bubble suspensions. *Physics of Fluids*, (submitted, 1996).
- Kassemi, M., Rashidnia, N., and Mercer, C., "Low-G and 1-G velocity and temperature fields in the vicinity of a bubble on a heated surface." *The Third Microgravity Fluid Physics Conference*, Cleveland, Ohio, June 1996.
- Koster, J.N. and Nguyen, K. Steady natural convection in a double layer of immiscible liquids with density inversion. *Int. J. Heat Mass Transfer*, vol. 39, 467-478 (1996).
- Krall, A.H. and Weitz, D.A. "Dynamic Light Scattering from Colloidal Gels." *Proceedings of the Third NASA Conference on Fluid Physics*, NASA CP 3338, pp.403 & 407, Cleveland, OH, June 13-15, 1996.
- Kugler, S. and Dhir, V.K., "Enhancement of nucleate boiling heat flux on macro/micro structured surfaces cooled by multiple impinging jets." *AIChE Symposium Series*, vol. 92, pp. 287-293, August 3-6, 1996.
- LaCasse, M.-D., Grest, G.S., Levine, D., Mason, T.G., and Weitz, D.A., A model for the elasticity of compressed emulsions. *Phys. Rev. Lett.*, 76, 3448-3451 (1996).

Ladd, A.J.C., Gang, H., Zhu, J.X., and Weitz, D.A. Temporal and spatial dependence of hydrodynamic correlations: simulation and experiment. *Phys. Rev. E*, 52, 6550-6572 (1995).

Larsson, R., Runesson, K., and Sture, S. Embedded Localization Band in Undrained Soil Based on Regularized Strong Discontinuity - Theory and FE analysis. *Int. J. Solids and Structures*, vol. 33, no. 20, 3081-3101 (1996).

Lee, H.S., and Merte, H., Jr., "The origin of the dynamic growth of vapor bubbles associated with vapor explosions." 1996 ASME International Congress and Exposition, in Atlanta, GA, for session "Nov. 17-22, 1996.

Lee, H.S., Merte, H., Jr., Spherical vapor bubble growth in uniformly superheated liquids. *Int. J. Heat Mass Transfer*, (1996).

Lee, H.S., Merte, H., Jr., Hemispherical vapor bubble growth in microgravity: experiments and model. *Int. J. Heat Mass Transfer*, (1996).

Lee, H.S., Merte, H., Jr., and Chiaramonte, F., "The pool boiling curve in microgravity." AIAA conference in Reno, NV, January 15, 1996.

Lempert, W.R., Harris, S.R., Hersch, L., Burcham, C.L., Miles, R.B., Gee, K., Haugland, R.P., and Saville, D.A. "Quantitative flow visualization of internal circulation in droplets by phantom flow tagging." American Institute of Aeronautics and Astronautics, 1995 AIAA Meeting, Paper AIAA-95-0168, Reno Nevada, January 1996.

Lin, J. Kamotani, Y., Ostrach, S., An experimental study of free surface deformation in oscillatory thermocapillary flow. *Acta Astronautica*, vol. 35, (November 18, 1995).

Liu, A.J., Ramaswamy, S., Mason, T.G., Gang, H., and Weitz, D.A., Anomalous viscous loss in emulsions. *Phys. Rev. Lett.*, 76, 3017-3020 (1996).

Liu, J., "Chain dynamics in a dilute magnetorheological fluid." Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, 6/13-6/15, 1996.

Liu, J., and Hagenbuechle, M., "Chain dynamics in a dilute magnetorheological fluid." Proceedings at Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June, 13-15, 1996.

Mason, T.G. and Weitz, D.A., Linear viscoelasticity of colloidal hard sphere suspensions near the glass transition. *Phys. Rev. Lett.*, 75, pp. 2770-2773 (1995).

Mason, T.G., Bibette, J., and Weitz, D.A., Yielding and flow of monodisperse emulsions. *J. Colloid Interfac. Sci.*, 179, 439-448 (1996).

Mason, T.G., Krall, A.H., Gang, H., Bibette, J., and Weitz, D.A., Monodisperse emulsions: properties and uses. *Encyclopedia of Emulsion Technology*, P. Becher, Ed., vol. 4, 299 (1996).

Mason, T.G., Krall, A.H., Gang, H., Bibette, J., and Weitz, D.A., Monodisperse emulsions: properties and uses. *Encyclopedia of Emulsion Technology*, P. Becher, Ed., vol. 4, 299 (1996).

Masud, J., Kamotani, Y., and Ostrach, S., Oscillatory thermocapillary flow in cylindrical columns of high prandtl number fluids. *Journal of Thermophysics and Heat Transfer*, (1996).

McQuillen, J., Observations of gas-liquid flows through contractions in microgravity. NASA Conference Publication, 3338, pp. 95-102 (1996).

Merte, H., Jr., "An overview of the microgravity environment and its effects on science." presented at AIAA 34th Aerospace Sciences Meeting, AIAA Paper 96-0401, Jan. 15-18, 1996, Reno, NV.

Merte, H., Jr., Lee, H.S., "Homogeneous nucleation in microgravity at low heat flux: experiments and theory." presented at Symposium "Heat Transfer in Microgravity Systems, 1995 International Mechanical Engineering Congress and Exposition" ASME Paper 95-WA/HT-41, San Francisco, CA, Nov. 13-17, 1995.

- Merte, H., Jr., Lee, H.S., Homogeneous nucleation in microgravity at low heat flux: experiments and theory. *J. of Heat Transfer.*, (1996).
- Mukhin, S.I., Kyung, B., and Ferrell, R.A., Spin-fluctuation gating in the c-axis non-Drude conductivity of the high T_c cuprates. *Annalen der Physik*, (1996).
- Ostrach, S., "Surface tension driven convection experiment." presented at the 27th AIAA Fluid Dynamics Conference, New Orleans, LA, June 17-20, 1996.
- Ostrach, S. and Kamotani, Y., Surface tension driven convection experiment (STDCE)," NASA Contractor Report 198476. NASA Tech Brief, (June 1996).
- Ostrach, S. and Kamotani, Y., "Surface tension driven convection experiment-2." Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 13-15, 1996.
- Ostrach, S., Kamotani, Y., and Pline, A., "Oscillatory thermocapillary flows." presented at Fluids in Space, Naples, Italy, April 22-26, 1996.
- Page, J.H., Schriemer, H.P., Bailey, A.E., and Weitz, D.A., Experimental test of the diffusion approximation for multiply scattered sound. *Phys. Rev. E*, 52, 3106-3114 (1995).
- Page, J.H., Sheng, P., Schriemer, H.P., Jones, I., Jing, X., and Weitz, D.A., Group velocity in strongly scattering media. *Science*, 271, 634-637 (1996).
- Prakash, A. and Koster, J.N. Steady Rayleigh-Benard convection in a two-layer system of immiscible liquids. *J. Heat Transfer*, vol. 118, no. 2, 366-373 (1996).
- Prakash, A. and Koster, J.N. Steady natural convection in a GaAs melt encapsulated by molten B_2O_3 . *J. Material Synthesis and Processing*, vol. 4, no. 1, 43-50 (1996).
- Rame, E., "Physics of liquid spreading." Pennsylvania State U., March, 1996.
- Rame, E., "Hydrodynamics near moving contact lines." Carnegie Mellon Polymer Symposium, May, 1996.
- Rame, E., "Hydrodynamics of moving contact lines." Institute for paper science and technology, May, 1996.
- Rame, E., "Microscale hydrodynamics near moving contact lines." Third Fluids Microgravity Conference, NASA LeRC, Cleveland, OH, June, 1996.
- Rame, E., and Garoff, S., Microscopic and macroscopic dynamic interface shapes and the interpretation of dynamic contact angles. *J. Colloid Interface Sci.*, vol. 177, 234 (1996).
- Runesson, K., Peric, D., and Sture, S. Effect of Pore Fluid Compressibility on Localization in Elastic-Plastic Porous Solids under Undrained Conditions. *Int. J. Solids and Structures*, vol. 33, no. 10, 1501-1518 (1996).
- Rutgers, M.A., Dunsmuir, J., Russel, W.B., and Chaikin, P.M., Hard sphere equation of state. *Science*, (1995).
- Rutgers, M.A., Russel, W.B., Chaikin, P.M., and Dunsmuir, J.H., Real hard spheres. *American Physical Society*, vol. 40, no. 1, (1995).
- Rutgers, M.A., Xue, J.Z., Herbolzheimer, E., Russel, W.B., and Chaikin, P.M., Crystalline fluidized beds. *Physical Review E*, 51, 4674 (1995).
- Shen, X.F., Anilkumar, A.V., Grugel, R.N., and Wang, T.G. Utilizing vibration to promote microstructure homogeneity in crystals during floating-zone processing. *J. Crystal Growth*, in press, (1996).
- Shi, W. and Apfel, R. Deformation and position of acoustically levitated liquid. *J. Acoust. Soc. Am*, vol 94, 1977-1984 (1966).

- Shi, W.T., Apfel, R. E. and Holt, R. G. The instabilities of liquid drops in sound field. *Phys. of Fluids*, Vol 7, no. 11, 2601-2607 (1995).
- Son, G. and Dhir, V.K., "Numerical simulation of liquid-vapor, liquid-gas, liquid-liquid interfaces subjected to Taylor instability." Presented at the Fluid Engineering Conference of ASME, July -8-12, 1996.
- Son, G. and Dhir, V.K., "Non-linear Taylor instability with application to film boiling and melting." *Proceedings of the Japan-US Seminar on Two Phase Flow*, pp.301-309, July 15-20, 1996.
- Spiegelberg, S.H., Ables, D.C. and McKinley, G.H., The role of end-effects on measurements of extensional viscosity in viscoelastic polymer solutions with a filament stretching rheometer. *J. Non-Newtonian Fluid Mech.*, vol. 64, 229-267 (1996).
- Spiegelberg, S.H. and McKinley, G.H., "Elastic and viscous contributions to stress in extensional rheometry of viscous polymer solutions." *Proc. XIIth Int. Congr. on Rheology*, Quebec City, Canada, vol.1, 211, 1996.
- Spiegelberg, S.H. and McKinley, G.H., Stress relaxation and elastic decohesion of viscoelastic polymer solutions in extensional flow. *J. Non-Newtonian Fluid Mech.*, (1996).
- Spiegelberg, S.H., and McKinley, G.H., "The extensional rheology of non-newtonian materials." *Proc. from the Third Microgravity Fluid Physics Conference*, NASA LeRC, Cleveland, OH, 1996.
- Tian, Y., Holt, R.G., and Apfel, R. E. Investigations of liquid surface rheology of surfactant by droplet shape oscillations. *Phys. of Fluids*, 7 (12), 2938-2949 (1996).
- Wang, T.G., Anilkumar, A.V., and Lee, C.P. Oscillations of liquid drops: Results from USML-1 experiments in space. *J. Fluid Mech*, vol. 308, 1-14 (1996).
- Weitz, D.A., Materials: foams flow by stick and slip. *Nature*, 381, 476 (1996).
- Weitz, D.A., "Complex fluids: Science, technology and microgravity." *Proceedings of the Third NASA Conference on Fluid Physics*, NASA CP 3338, pp. 25-26, Cleveland OH, June 13-15, 1996.
- Weitz, D.A. and Ladd, A.J.C., Response to comment. *Phys. Rev. Lett.*, 75, 2253 (1995).
- Zhu, J.X., Phan, S.E., Russel, W.B., Chaikin, P.M., Absorption of tetralin by PMMA spheres in decalin/tetralin mixture. *American Physical Society*, vol. 40, no. 1, (1995).

Flight: Fundamental Physics

- Adriaans, M.J., Moeur, W.A., Boyd, S.T.P., Strayer, D.M., and Duncan, R.V. Cryogenic design of the liquid helium experiment 'Critical Dynamics in Microgravity'. *Cryogenics*, vol. 36, 787 (1996).
- Barmatz, M., and Hahn, I. "Measurements near the liquid-gas critical point of ^3He ." *Proceedings of the 21st International Low Temperature Physics Conference LT-21 (Prague)*, Czechoslovak Journal of Physics 46 (1996).
- Barmatz, M. and Hahn, I. "Measurements near the liquid-gas critical point of ^3He ." *Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop*, NASA Document D-13845 (1996).
- Duncan, R., Boyd, S., Moeur, W., Robinson, S., Akau, R., and Gianoulakis, S. Critical Dynamics in Microgravity. *International Journal of Thermophysics*, vol. 17, 631 (1996).
- Everitt, C.W.F. "Update on MiniSTEP." *International Workshop of the Fundamental Physics Advisory Group*, Headquarters of the European Space Agency, Paris, France, April, 1996.
- Everitt, C.W.F. "Satellite Test of the Equivalence Principle (STEP)." *9th Russian Gravitational Conference*, Novgorod, Russia, June, 1996.
- Everitt, C.W.F. "The NASA/ESA miniSTEP Experiment." *COSPAR*, Birmingham, U.K., July 7, 1996.

- Gammon, R.W., "Development and flight of the Zeno experiment at the University of Maryland." invited paper at the Human Exploration & Development of Space Conference, University of Maryland, November 8, 1995.
- Gammon, R.W., Shaumeyer, J.N., Briggs, M.E., Boukari, H., and Gent, D.A., "Zeno: critical fluid light scattering experiment." paper #43 at the Third Microgravity Fluid Physics Conference, June 13-15, 1996.
- Gammon, R.W., Shaumeyer, J.N., Briggs, M.E., Boukari, H., and Gent, D.A., "Zeno: comparison of critical fluctuation PCS on Earth and in low gravity." paper at the Photon Correlation and Scattering Topical Meeting, Optical Society of America, Capri, Italy, August 1996.
- Gammon, R.W., Shaumeyer, J.N., Briggs, M.E., Boukari, H., and Gent, D.A., "Zeno: critical fluid light scattering in microgravity." invited paper at the NATO Advanced Research Workshop, Jagiellonian University, Krakow, Poland, August 1996.
- Lipa, J. A. "Critical phenomena in microgravity: past, present, and future." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13845, 8-12 (1996).
- Liu, F. C., Duncan, R., Israelsson, U., Chui, T., Hensinger, D., Nash, A., Adriaans, M., and Moeur, W. "Effect of gravity on thermal conductivity measurement of 4He near Tl." Proceedings of the 21st International Conference on Low Temperature Physics LT-21 (Prague), Czechoslovak Journal of Physics, vol. 46, Supplement S1, 87 (1996).
- Nash, A.E., Mukharsky, Y.M., Aaron, K.M., and Paine, C.G. "Development of structural and thermal elements for Critical Dynamics in Microgravity Experiment." Proceedings of the 35th Aerospace Sciences Meeting, Reno, NV (1996).
- Palik, E.D., Boukari, H., and Gammon, R.W., Experimental study of the effect of surface defects on the finesse and contrast of a Fabry-Perot interferometer. Appl. Optics, 35, pp. 38-50 (1996).
- Palik, E.D., Boukari, H., and Gammon, R.W., Experimental study of the effect of surface defects on the finesse and contrast of a Fabry-Perot interferometer. Appl. Optics, 35, pp. 38-50 (1996).
- Rudnick, J., and Barmatz, M. "Electric fields near the liquid-vapor critical point." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA Document D-13845 (1996).
- Sapilewski, G. "Differential accelerometer testing apparatus." Symposium on Fundamental Physics in Space, London, October 1995.
- Swanson, D. R., Nissen, J. A., Qin, X., Lipa, J. A., Chui, T. C. P., Israelsson, U. E., and Gasparini, F. M. "Heat capacity of confined helium very near the lambda point." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13845, 13-16 (1996).
- Torii, R. "SQUID position sensor for the Stanford accelerometer." Symposium on Fundamental Physics in Space, London, October 1995.
- Worden, P. "The MiniSTEP experiment." MiniSTEP 'New Ideas' Session, Jet Propulsion Laboratory, May 1996.
- Worden, P. "The equivalence principle experiment on MiniSTEP." International Scientific Workshop, European Space Agency Headquarters, Paris, April 1996.
- Worden, P. "Testing the equivalence principle in space." 1996 April Meeting of the American Physical Society, Indianapolis, May 1996.
- Worden, P. "Accelerometer development at Stanford." Symposium on Fundamental Physics in Space, London, October 1995.
- Zhang, K.J., Briggs, M.E., Gammon, R.W., and Sengers, J.V., Optical measurement of the Soret coefficient and the diffusion coefficient of liquid mixtures. J. Chem. Phys., 104, pp. 6881-6892 (1996).

Flight: Materials Science

Abbaschian, R. and Coriell, S.R. "In situ monitoring of crystal growth using MEPHISTO." NASA Microgravity Materials Science Conference, NASA # LP 3342, pp. 71-76, October, 1996.

Abbaschian, R. Gokhale, A.B., and Allen, D.B. "A study of directional solidification of faceted Bi-Sn alloys in microgravity." Solidification Science and Processing, ed. Ohnaka, I. and Stefanescu, D.M., TMS, pp. 73-84, 1996.

Alexander, J.I.D. Estimation of experiment sensitivity to residual acceleration. Microgravity Quarterly, vol. 5, (1995).

Alexander, J.I.D. "Response of Crystal Growth Experiments to Time-Dependent Residual Acceleration." Lecture Notes in Physics, Vol. 464, L. Ratke, H. Walter, and B. Feuerbacher, eds., pp 95-105, Springer Verlag, Berlin, 1996.

Alexander, J.I.D., and Fedoseyev, A. "Simulation of steady and unsteady low-g transport during solidification (poster presentation)." 31st Annual COSPAR meeting, Birmingham, England, July 14-21, 1996.

Andrews, J.B. "Coupled Growth in Hypermonotectics." Extended Abstract, Microgravity Materials Science Conference, Report Summaries Volume, pp 30-31, 1996.

Andrews, J.B. "Coupled Growth in Hypermonotectics." Microgravity Materials Science Conference, Huntsville, Alabama. June 10-11, 1996.

Andrews, J.B., Hayes, L.J., Arikawa, Y., and Coriell, S.R. Microgravity Processing of Immiscible Aluminum-Indium Alloys. Advances in Space Research, (accepted for publication).

Andrews, J.B., Hayes, L.J., Arikawa, Y., and Coriell, S.R. "Microgravity Processing of Immiscible Aluminum-Indium Alloys." 31st Scientific Assembly of COSPAR, Birmingham, England, July 14-21, 1996.

Andrews, J.B., Hayes, L.J., Arikawa, Y., O'Dell, J.S., and Cheney, A. "Coupled Growth in Immiscible Alloys." Annual Meeting of the International Society for Optical Engineering SPIE, Denver, Colorado, August 4-5, 1996.

Andrews, J.B., Hayes, L.J., Arikawa, Y., O'Dell, J.S., and Cheney, A.B. Microgravity Solidification of Immiscible Alloys. Materials Science Forum (Transtec Publications, Roosz and Rettenmayr, eds.), 50-66 (1996).

Andrews, J.B., Hayes, L.J., Arikawa, Y., O'Dell, S., and Cheney, A. "Coupled Growth in Immiscible Alloys." Proceedings ("Space Processing of Materials") of the Annual Meeting of the International Society for Optical Engineering-SPIE, V2809 N. Ramachandran, ed., 12-22 (1996).

Andrews, J.B., O'Dell, J.S., Cheney, A.B., Arikawa, Y., and Hayes, L.J. "Ampoule Design and Testing for Microgravity Experimentation on Coupled Growth in Hypermonotectics." Proceedings of the 8th International Conference on Experimental Methods for Microgravity Materials Science, a publication of the Minerals, Metals and Materials Society,

Andrews, J.B., O'Dell, J.S., Cheney, A.B., Arikawa, Y., and Hayes, L.J. "Ampoule Design and Testing for Microgravity Experimentation on Coupled Growth in Hypermonotectics." TMS Annual Meeting, Anaheim, California, February 5-8, 1996.

Arikawa, Y., Andrews, J.B., Coriell, S.R., and Mitchell, W.F. "Numerical Simulation of Directional Solidification of Hypermonotectic Alloys." Proceedings of the 8th International Conference on Experimental Methods for Microgravity Materials Science, a publication of the Minerals, Metals and Materials Society, R.S. Schiffman, ed., 1996.

Arikawa, Y., Andrews, J.B., Coriell, S.R., and Mitchell, W.F. "Numerical Simulation of Directional Solidification of Hypermonotectic Alloys." TMS Annual Meeting, Anaheim, California, February 5-8, 1996.

Arnold, W., Matthiesen, D., Bennett, R., and Jayne, D., An innovative method for preparing semiconductor charges used in crystal growth and shear cell diffusion experiments. J. of Crystal Growth, (accepted 1996).

Bachmann, K.J., Dietz, N., Miller, A., Höpfner, C., Scroggs, J.S., Tran, H.T., Kepler, G., Ito, K., and Banks, H.T. "Real-time Monitoring of Chemical Vapor Deposition Processes: Effects of Pressure and Flow." 17th Int. Union of Crystallogr. Congress, Seattle, Washington, August 1996.

Bachmann, K.J., Höpfner, C., Sukidi, N., Miller, A.E., Harris, C., Aspnes, D.E., Dietz, N., Tran, H.T., Beeler, S., Ito, K., Banks, H.T., and Rossow, U. "Molecular Layer Epitaxy by Real-Time Optical Process Monitoring." ALE-4 Conference, Linz, Austria, July 1996.

Banish, R.M., Alexander, J.I.D., Jalbert, L.B., and Rosenberger, F. "In situ radiotracer diffusion measurement technique (invited paper)." Gravitational Effects in Fluid and Materials Science Commission Meeting, 31st COSPAR Scientific Assembly, Birmingham, England, July 1996.

Banish, R.M., Jalbert, L.B., Roberson, R.J., and Rosenberger, F. "In situ radiotracer diffusion measurement technique (invited paper)." Space Processing of Materials Symposium, 1996 SPIE, Denver, Colorado, August 1996.

Barber, P., Fripp, A., Debnam, W., Berry, R., and Simchick, R. Growth rates and interface shapes in germanium and lead tin telluride observed in-situ, real time in vertical Bridgman furnaces. J. Crystal Growth, vol. 147, 83-90 (1995).

Bose, A., and German, R.M., "Developments in the sintering of Tungsten heavy alloys." Proceedings of the Sintering Technology, R. M. German, G. L. Messing and R. G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 269-276, 1996.

Bose, A., and German, R.M., Developments in the sintering of Tungsten heavy alloys. Sintering Technology, R.M. German, G.L. Messing and R.G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 269-276 (1996).

Brebrick, R.F., and Fang, R. CdTe II: Defect Chemistry. J. Phys. Chem. Solids, vol. 57, 451-460 (1996).

Brebrick, R.F., and Liu, H. Partial Pressures of Zn and Se₂ over ZnSe(s) from Optical Density Measurements. High Temperature and Materials Science, vol. 35, 215-237 (1996).

Bune, A.V., Gillies, D.C., and Lehoczy, S.L. "Evaluation of Temperature Gradient in Advanced Automated Directional Solidification Furnace (AADSf) by Numerical Simulation." Proceedings of SPIE - The International Society for Optical Engineering - 1996 International Symposium on Space Processing of Materials, Denver, Colorado, August 4-6, 1996, vol.

Bune, A.V., Gillies, D.C., and Lehoczy, S.L. "Optimization of Bulk HgCdTe Growth in a Directional Solidification Furnace by Numerical Simulation." Mat. Res. Soc. Symp. Proceedings, vol. 398, 139-144 (1996).

Bune, A.V., Gillies, D.C., Watring, D.A., and Lehoczy, S.L. "Modeling of Convection and Segregation During HgCdTe Directional Solidification with Emphasis on Coupling with Crystal-Melt Interface Alteration." Tenth American Conference on Crystal Growth, Vail, Colorado, August 4-9, 1996.

Busch, R., Kim, Y.J., Johnson, W.L., Rulison, A.J., and Rhim, W.K. "Determination of the specific heat capacity and the total hemispherical emissivity of the deeply undercooled Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni₁₀Be_{22.5} alloy." Proc. of the 7th Int'l. TMS Symposium on Experimental Methods for Microgravity Materials Science, TMS, 15-21 (1995).

Busch, R., Kim, Y.J., Johnson, W.L., Rulison, A.J., and Rhim, W.Q. Total hemispherical emissivity and specific heat capacity of deeply undercooled Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni₁₀Be_{22.5} melts. Appl. Phys. Lett., vol. 66, 3111-3113 (1995).

Busch, R., Kim, Y.J., Schneider, S., and Johnson, W.L. "Atom Probe Field Ion Microscope and Levitation Studies of the Decomposition and Crystallization of Undercooled Zr-Ti-Cu-Ni-Be Melts." ISMANAM-95 Conference Proceedings, Materials Forum, 77-82 (1996).

Bushnell, L.T., Koss, M.B., LaCombe, J.C., and Glicksman, M.E., Use of microgravity to interpret dendritic growth kinetics at small supercoolings. J. Crystal Growth, (submitted 1996).

Carlson, F.M., Lee, T., Moosbrugger, J.C., and Larson, Jr., D.J. "Thermomechanical Analysis in Directional Solidification of CdTe." Space Processing of Materials Session, SPIE, Denver, Colorado, August 4-5, 1996.

Carlson, F.M., Lee, T., Moosbrugger, J.C., and Larson, Jr., D.J. "Thermomechanical Analysis in Directional Solidification of CdTe." Space Processing of Materials, SPIE Proceedings vol. 2809, N. Ramachandran, ed., pp 185-195, Denver, Colorado, August 4-5, 1996.

Chen, K.T., and Wiedemeier, H. The Temperature-Composition Phase Diagram and the Miscibility Gap of Hg_{1-x}Cd_xTe Solid Solutions by Dynamic Mass-Loss Measurements. J. Electronic Materials, vol. 24, 405-411 (1995).

Chung, H., Chung, H., Raghothamachar, B., and Larson, Jr., D.J. "Synchrotron White Beam X-Ray Topography Characterization of Structural Defects in Microgravity and Ground Based CdZnTe crystals." SPIE Meeting Symposium on Space Processing of Materials, Denver, Colorado, August 4-9, 1996.

Chung, H., Dudley, M., and Larson, Jr., D.J. "Imaging Large CdZnTe Single Crystals by Synchrotron White Beam X-ray Topography." National Synchrotron Light Source Activity Report 1994, E.Z. Rothman, ed., BNL, Associated Universities, Inc., p B125, 1995.

Chung, H., Dudley, M., and Larson, Jr., D.J. "Synchrotron White Beam X-ray Topographic Investigation of Microgravity Grown CdZnTe Single Crystals." National Synchrotron Light Source Activity Report 1994, E.Z. Rothman, ed., BNL, Associated Universities, Inc., p B126, 1995.

Chung, H., Raghothamachar, B., Dudley, M., and Larson, Jr., D.J. "Synchrotron White Beam X-Ray Topography Characterization of Structural Defects in Microgravity and Ground Based CdZnTe crystals." SPIE, Space Processing of Materials, 1996.

Chung, H., Raghothamachar, B., Dudley, M., and Larson, Jr., D.J. "Synchrotron White Beam X-Ray Topography Characterization of Structural Defects in Microgravity and Ground Based CdZnTe crystals." Space Processing of Materials, SPIE Proceedings vol. 2809, N. Ramachandran, ed., pp. 45-56, Denver, Colorado, August 4-5, 1996.

Chung, H., Raghothamachar, B., Dudley, M., and Larson, Jr., D.J. "Synchrotron White Beam X-Ray Topography Characterization of Structural Defects in Microgravity and Ground Based CdZnTe Crystals." SPIE Proceedings, vol. 2809, Space Processing of Materials, 1996.

Chung, H., Raghothamachar, B., Wu, J., Dudley, M., Larson, Jr., D.J., and Gillies, D.C. "Characterization of Growth Defects in CdZnTe Single Crystals by Synchrotron White Beam X-Ray Topography." Materials Research Society Symposium Proceedings, vol. 378, Defect and Impurity Engineered Semiconductors and Devices, S. Ashok, J. Chevallier,

Chung, H., Raghothamachar, B., Wu, J., Dudley, M., Larson, Jr., D.J., and Gillies, D.C. "Characterization of Growth Defects in CdZnTe Single Crystals by Synchrotron White Beam X-ray Topography." Mat. Res. Soc. Symp. Proc. (in "Defect and Impurity-Engineered Semiconductors and Devices"), S. Ahok, J. Chevallier, I. Akasaki, N.M. Johnson, and

Chung, H., Wu, J., Dudley, M., and Larson, Jr., D.J. "Characterization of Growth Defects in an Ultra-Thin CdZnTe Single Crystal by Synchrotron White Beam X-ray Topography." National Synchrotron Light Source Activity Report 1994, E.Z. Rothman, ed., BNL, Associated Universities, Inc., p B125, 1995.

Coriell, S.R., Murray, B.T., Chernov, A.A., and McFadden, G.B. Effects of shear flow and anisotropic kinetics on the morphological stability of a binary alloy. Metalurgical and materials Transactions, vol. 27A, 687-694 (1996).

Curreri, P.A., and Kauckler, W.F. Real-time x-ray transmission microscopy of solidifying Al-In alloys. Met. Trans., vol. 27A, 801-808 (1996).

Dhindaw, B.K., Ganguly, P., Juretzko, F.R., and Stefanescu, D.M. "Particle redistribution during remelting of Al/SiC_p composites - an experimental and computational study." Annual TMS meeting and exhibition, R. Schiffman, ed., Anaheim, California, February 1996.

Dudley, M. "Combined Synchrotron White Beam X-ray Topography and High Resolution Triple Axis X-ray Diffraction Characterization and Analysis of Crystals Grown in Microgravity and Ground-Based Environments." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Dudley, M. "Applications of Synchrotron White Beam X-ray Topography in the Semiconductor Industry." 2nd International Workshop on Semiconductor Research Using Synchrotron Radiation, March 14-15, 1996.

Dudley, M., Larson Jr., D.J., Chung, H., and Raghothamachar, B. "Characterization of Zn-Alloyed CdTe Compound Semiconductors Processed in Microgravity on USML-1 and USML-2." 31st COSPAR Scientific Assembly, Birmingham, England, July 14-21, 1996.

Dudley, M., Larson, Jr., D.J., Chung, H., and Raghothamachar, B. "Characterization of Zn-alloyed CdTe Compound Semiconductors Processed in Microgravity on USML-1 and USML-2." COSPAR.

Dudley, M., Larson, Jr., D.J., Chung, H., and Raghothamachar, B. "Characterization of Zn-Alloyed CdTe Compound Semiconductors Processed in Microgravity on USML-1 and USML-2." Proceedings of 31st COSPAR Scientific Assembly, Birmingham, England, July 14-21, 1996.

Egry, I., Jacobs, G., Schwartz, E., and Szekely, J. Surface Tension Measurements of Metallic Melts Under Microgravity. *International Journal of Thermophysics*, vol. 17, no. 5, 1181-1189 (1996).

Fang, R., and Brebrick, R.F. CdTe I: Solidus Curve and Composition-Temperature-Tellurium Partial Pressure Data for Te-Rich CdTe(s) from Optical Density Measurements. *J. Phys. Chem. Solids*, vol. 57, 443-450 (1996).

Fedoseyev, A., and Alexander, J.I.D. An Inverse Finite Element Method for Pure and Binary Solidification Problems. *J. Computational Physics*, (1996, accepted).

Flemings, M.C., Trapaga, G., and Hyers, R. "The Measurement of the Viscosity and Surface Tension of Undercooled Melts under Microgravity Conditions and Supporting MHD Calculations." Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.

Fripp, A.L., Debnam, W.J., Rosch, W.R., and Narayanan, R. "The effect of microgravity direction on the growth of PbSnTe." Presented at The Tenth American Conference on Crystal Growth, August 4-9, 1996, Vail, CO.

Ge, Y.R., and Wiedemeier, H. Characteristics of Island Growth of $Hg_{1-x}Cd_xTe$ on (100) CdTe Substrates by Chemical Vapor Transport. *J. Electronic Materials*, vol. 25, 1067-1071 (1996).

German, R.M., Grain agglomeration in solid-liquid mixtures under microgravity conditions. *Metallurgical and Materials Transactions*, vol. 26B, pp. 649-651 (October 1995).

German, R.M., "The microstructures of liquid phase sintered materials." Proceedings of the Sintering Technology, R.M. German, G.L. Messing and R.G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 213-220, 1996.

German, R.M., "The microstructures of liquid phase sintered materials." presented at Sintering 1995, Penn State University, University Park, PA, September 25, 1995.

German, R.M., "Gravitational effects in liquid phase sintering." submitted presentation, 1996 TMS Annual Meeting, Anaheim, CA, February 6, 1996.

German, R.M., "Recent advances in liquid phase sintering." invited colloquium, Department of Materials Science and Engineering, Case Western Reserve University, Cleveland, OH, April 1, 1996.

German, R.M., "Sintering processes in novel manufacturing systems." invited presentation, Institute of Mechanics and Materials, University of California, San Diego, CA, May 14, 1996.

German, R.M., "The gravitational role in liquid phase sintering." presented at the Microgravity Materials Science Conference, Huntsville, AL, June 11, 1996.

German, R.M., "Grain agglomeration and coalescence in liquid phase sintering." presented at 1996 World Congress on Powder Metallurgy and Particulate Materials, Washington, DC, June 17, 1996.

German, R.M., "Calculation and observation of sintering shrinkage and distortion." presented at the 1996 International Powder Injection Molding Symposium, Penn State Scanticon, State College, PA, August 27, 1996.

German, R.M., Grain agglomeration in solid-liquid mixtures under microgravity conditions. *Metallurgical and Materials Transactions*, vol. 26B, pp. 649-651 (October 1995).

German, R.M., The microstructures of liquid phase sintered materials. *Sintering Technology*, R.M. German, G.L. Messing and R.G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 213-220 (1996).

German, R.M. and Liu, Y., Grain agglomeration in liquid phase sintering. *Journal of Materials Synthesis and Processing*, vol. 4, pp. 23-34 (1996).

German, R.M. and Liu, Y. Grain agglomeration in liquid phase sintering. *Journal of Materials Synthesis and Processing*, vol. 4, pp. 23-34 (1996).

German, R.M., Liu, Y., and Griffo, A., Gravitational effects on grain coarsening during liquid phase sintering. *Metallurgical and Materials Transactions*, (1996).

German, R.M., Liu, Y., and Griffo, A., Gravitational effects on grain coarsening during liquid phase sintering. *Metallurgical and Materials Transactions*, (1996).

Gillies, D.C., Lehoczky, S.L., Szofran, F.R., Watring, D.A., and Alexander, H.A. Effects of Residual Accelerations during Microgravity Directional Solidification of Mercury Cadmium Telluride on the USMP-2 Mission. *J. Crys. Growth* (in press).

Gillies, D.C., Lehoczky, S.L., Szofran, F.R., Watring, D.A., and Alexander, H.A. "Effect of Residual Acceleration during Microgravity Directional Solidification of Mercury Cadmium Telluride on the USMP-2 Mission." Tenth American Conference on Crystal Growth, Vail, Colorado, August 4-9, 1996.

Gillies, D.C., Reeves, F.A., Jeter, L.B., Sledd, J.D., Cole, J.M., and Lehoczky, S.L. "The Advanced Automatic Directional Solidification Furnace." *Proceedings of SPIE - The International Society for Optical Engineering - 1996 International Symposium on Space Processing of Materials*, Denver, Colorado, August 4-6, 1996, vol. 2809, 329-335 (1996).

Glicksman, M.E., "Dendritic growth studies on the space shuttle." *Science Update*, at the Sixth Eastern Regional Conference on Crystal growth, ACCG/east-95, in Atlantic City, NJ, October, 1995.

Glicksman, M.E., "The experimental measurement of the thermal expansion of liquid succinonitrile." October meeting of the Mohawk chapter of the TMS, October, 1995.

Glicksman, M.E., "Convective effects in microgravity on dendritic growth kinetics and morphology." 34th Aerospace Sciences Meeting and Exhibit, Reno, NV, January, 1996.

Glicksman, M.E., "Development of a university based local teleoperations site for the performance of experiments in microgravity." 8th International Symposium on Experimental Methods for Microgravity materials Science at the 5th TMS Annual Meeting, Anaheim, CA, February, 1996.

Glicksman, M.E., "Diffusion-limited dendritic growth." *Current Status and Recent Microgravity Results*, Chemical Engineering Seminar, University of Florida, April, 1996.

Glicksman, M.E., "Experience with a materials microgravity space flight experiment." URI Composite Materials Program, Rensselaer Polytechnic Institute, Troy, NY, April, 1996.

Glicksman, M.E., "Study of dendritic crystal growth in microgravity using teleoperational control." *Space Processing of Materials*, SPIE's 1996 International Symposium on Optical Science, Engineering, and Instrumentation, Denver, CO, August, 1996.

Glicksman, M.E., "Use of microgravity to interpret dendritic growth kinetics at small supercoolings." Tenth American Conference on Crystal Growth (ACCG-10), Vail, CO, August, 1996.

Glicksman, M.E., Koss, M.B., Bushnell, L.T., LaCombe, J.C., and Winsa, E.A., "Dendritic growth measurements in microgravity." *Lecture Notes in Physics*, vol. 464, Eds. L. Ratke, H. Walter, and B. Feuerbacher, (Springer-Verlag, Berlin, p. 63, 1996).

Glicksman, M.E., Koss, M.B., Bushnell, L.T., LaCombe, J.C., and Winsa, E.A., "Convective effects in microgravity on dendritic growth kinetics and morphologies." Paper # AIAA 96-0251, Aerospace Sciences Meeting and Exhibit, Reno, NV, 1996.

Hayes, L.J., and Andrews, J.B. The Effect of Convective Instability on Coupled Growth of Hypermonotectic Alloys. *Materials Science Forum* (V215-216, Transtec Publications, Roosz and Rettenmayr, eds.), 283-290 (1996).

Hayes, L.J., and Andrews, J.B. "Convection in Hypermonotectic Alloys." TMS Annual Meeting, Anaheim, California, February 5-8, 1996.

- Hayes, L.J., and Andrews, J.B. "Convective Instability in Directionally Solidified Hypermonotectic Alloys (poster presentation)." 31st Scientific Assembly of COSPAR, Birmingham, England, July 14-21, 1996.
- Heaney, D.F., German, R.M. and Ahn, I.S., The gravitational effects on low solid-volume fraction liquid-phase sintering. *Journal of Materials Science*, vol. 30, pp. 5808-5812 (October 1995).
- Heaney, D.F., German, R.M., and Ahn, I.S., The gravitational effects on low solid- volume fraction liquid-phase sintering. *Journal of Materials Science*, vol. 30, pp. 5808-5812 (October 1995).
- Horton, M.R. "Implementation of a Single Crystal Viscoplastic Constitutive Model for CdTe into MARC Finite Element Code (M.S. thesis)." Clarkson University, Potsdam, New York, 1995.
- Iacocca, R.G., Liu, Y., and German, R.M., "Microstructural examination of Tungsten heavy alloys sintered in a microgravity environment." *Proceedings of the Advances in Powder Metallurgy and Particulate Materials*, vol. 1, Metal Powder Industries Federation, Princeton, NJ, pp. 4.239-4-4.249, October 1995.
- Iacocca, R.G., Liu, Y., and German, R.M., "Microstructural examination of Tungsten heavy alloys sintered in a microgravity environment." *Advances in Powder Metallurgy and Particulate Materials*, vol. 1, Metal Powder Industries Federation, Princeton, NJ, pp. 4.239-4-4.249, October 1995.
- J.C. LaCombe, J.C., "Dendrite tip shape characteristics." *Material Research Society Fall '95 Conference, Symposium C*, December, 1995.
- Johnson, J.L., and German, R.M., Theoretical modeling of densification during activated solid-state sintering. *Metallurgical and Materials Transactions*, vol. 27A, pp. 441- 450 (1996).
- Johnson, J.L., and German, R.M., Solid state contributions to densification during liquid phase sintering. *Metallurgical and Materials Transactions*, (1996).
- Johnson, J.L., and German, R.M., "Solid-state sintering in the presence of a liquid phase." *Proceedings of the Sintering Technology*, R.M. German, G.L. Messing and R.G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 237-244, 1996.
- Johnson, J.L., and German, R.M., Theoretical modeling of densification during activated solid-state sintering. *Metallurgical and Materials Transactions*, vol. 27A, pp. 441- 450 (1996).
- Johnson, J.L. and German, R.M., Solid-state sintering in the presence of a liquid phase. *Sintering Technology*, R.M. German, G.L. Messing and R.G. Cornwall (eds), Marcel Dekker, New York, NY, pp. 237-244 (1996).
- Johnson, J.L. and German, R.M., Solid state contributions to densification during liquid phase sintering. *Metallurgical and Materials Transactions*, (1996).
- Johnson, J.L., Upadhyaya, A., and German, R.M., "Effect of solubility on shape retention during liquid phase sintering." *Proceedings of the Advances in Powder Metallurgy and Particulate Materials*, vol. 1, Metal Powder Industries Federation, Princeton, NJ, pp. 4.219-4.228, October 1995.
- Johnson, J.L., Upadhyaya, A., and German, R.M., "Effect of solubility on shape retention during liquid phase sintering." *Advances in Powder Metallurgy and Particulate Materials*, vol. 1, Metal Powder Industries Federation, Princeton, NJ, pp. 4.219-4.228, October 1995.
- Johnson, W.L. "Fundamental Aspects of Bulk Metallic Glass Formation in Multicomponent Alloys." *Proceedings of ISMANAM-95*, R.S. Schulz, ed., Materials Forum, 35-49 (1996).
- Juretzko, F.R., Dhindaw, B.K., Sen, S., and Stefanescu, D.M. "The use of x-ray transmission microscopy in the evaluation of particle distribution in metal ceramic composites (extended abstract)." 3rd International Conference on Composite Engineering ICCE/3, p 421, New Orleans, Louisiana, July 1996.
- Juretzko, F.R., Stefanescu, D.M., Dhindaw, B.K., and Sen, S. "Interfacial Energy $\Delta\gamma$ - theoretical and experimental evaluation for metal-ceramic systems." *ASM-TMS materials week '96*, Cincinnati, Ohio, October 1996 (in print).

- Kim, Y.J., Busch, R., and Johnson, W.L. "Crystallization Kinetics of the Undercooled Liquid $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ Alloy During Containerless Electrostatic Levitation Processing." 8th Int. Symp. of Experimental Methods for Microgravity Materials Science, TMS, R.A. Schiffman, ed., in press (1996).
- Kim, Y.J., Busch, R., Johnson, W.L., Rulison, A.H., and Rhim, W.Q. Experimental Determination of a Time-Temperature-Transformation Diagram of the Undercooled $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ Alloy Using Containerless Electrostatic Levitation Processing. *Appl. Phys. Lett.*, vol. 68, 1057-1059 (1996).
- Koss, M.B., "The isothermal dendritic growth experiment." Microgravity Materials Science Conference, Huntsville, AL, June, 1996.
- Koss, M.B., Bushnell, L.T., LaCombe, J.C., and Glicksman, M.E., The effect of convection on dendritic growth under microgravity conditions. *Chem. Eng. Comm.*, (in press 1996).
- LaCombe, J.C., Koss, M.B., Bushnell, L.T., de Jager, K.D., and Glicksman, M.E., "Dendrite tip shape characteristics." *Mat. Res. Soc. Symp. Proc.* (Materials Research Society, Pittsburgh, PA, in press 1996).
- LaCombe, J.C., Oudemool, J.L., Koss, M.B., Bushnell, L.T., Bushnell, and Glicksman, M.E., Measurement of thermal expansion in liquid succinonitrile and pivalic acid. *J. Crystal Growth*, (in press 1996).
- Larson, Jr., D.J. "Orbital Processing of High-Quality Zn-Alloyed CdTe Compound Semiconductors." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.
- Larson, Jr., D.J. "Orbital Processing of High-Quality Zn-Alloyed CdTe Compound Semiconductors." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.
- Larson, Jr., D.J., Chung, H., and Raghothamachar, B. "Synchrotron Characterization of Zn-Alloyed CdTe Compound Semiconductors Processed in Microgravity on STS-50 and -73." IUCR Meeting, Seattle, Washington, August 10-17, 1996.
- Larson, Jr., D.J., Dudley, M., Chung, H., and Raghothamachar, B. "Synchrotron Characterization of Zn-Alloyed CdTe Compound Semiconductors Processed in Microgravity on STS-50 and -73." IUCR.
- Larson, Jr., D.J., Dudley, M., Chung, H., and Raghothamachar, B. "Synchrotron Characterization of Zn-Alloyed CdTe Compound Semiconductors Processed in Microgravity on STS-50 and -73." IUCR Proceedings, 1996.
- Lee, D.S., Hoffmeister, W., Bayuzick, R., and Johnson, W.L. "Noncontact AC Calorimetry: Specific Heat of Liquid $Nb_{40}Ni_{60}$ and $Ni_{24}Zr_{76}$ as Measured on IML-2." *Thermophysical Journal, Proc. of the 4th Asian Thermophysical Properties Conference*, 884-888 (1995).
- Lee, D.S., Uffelman, D., and Johnson, W.L. Noncontact AC calorimetry on undercooled alloys: Science and technology of rapid solidification and processing. *NATO ASI Series E - Applied Sciences* (M. Otonari, ed.), vol. 278, 327-337 (1995).
- Lee, T. "Finite Element Analysis of the Thermal and Stress Fields During Directional Solidification of Cadmium Telluride (Ph.D. thesis)." Clarkson University, Potsdam, New York, 1996.
- Lee, T.C., Moosbrugger, J.C., Carlson, F.M., and Larson, Jr., D.J. "Finite Element Analysis of Thermal and Stress Fields in the Directional Solidification of Cadmium Telluride." *Computational Mechanics '95*, S.N. Athuri, G. Yagawa, and T.A. Cruse, eds., vol. 1, Springer, New York, pp 556-561, 1995.
- Lehoczky, S.L., Szofran, F.R., and Gillies, D.C. "Growth of Solid Solution Single Crystals." Second United States Microgravity Payload: One Year Report, P.A. Curreri and D.E. McCauley, eds., NASA Technical Memorandum 4737, 90-134 (1996).
- Lehoczky, S.L., Szofran, F.R., Gillies, D.C., and Watring, D.A. "Growth of Solid Solution Single Crystals." *Proceedings of the 1996 Microgravity Materials Science Conference*. Huntsville, Alabama, June 10-11, 1996 (in press).
- Lehoczky, S.L., Szofran, F.R., Su, C.-H., Scripa, R.N., and Sha, Y.-G. "Crystal Growth of Selected II-VI Semiconducting Alloys by Directional Solidification." *Proceedings of the 1996 Microgravity Materials Science Conference*, Huntsville, Alabama, June 10-11, 1996 (in press).

- Li, W., and Patterson, D. Electronic and Formation Energies for Deep Defects in Narrow-Gap Semiconductors. *Phys. Rev B*, vol. 53, 15622-15630 (1996).
- Liu, Y. and German, R.M., Contact angle and solid-liquid-vapor equilibrium. *Acta Materialia*, vol. 44, pp. 1657-1663 (1996).
- Liu, Y. and German, R.M., "Relationship between contact angle and surface tensions." *Proceedings of the Sintering Technology*, R.M. German, G.L. Messing and R.G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 229-2236, 1996.
- Liu, Y. and German, R.M., Contact angle and solid-liquid-vapor equilibrium. *Acta Materialia*, vol. 44, pp. 1657-1663 (1996).
- Liu, Y., and German, R.M., Relationship between contact angle and surface tensions. *Sintering Technology*, R.M. German, G.L. Messing and R.G. Cornwall (eds.), Marcel Dekker, New York, NY, pp. 229-2236 (1996).
- Liu, Y., Iacocca, R.G. and German, R.M., "A challenge to liquid phase sintering concepts." *Proceedings of the Advances in Powder Metallurgy and Particulate Materials*, vol. 1, Metal Powder Industries Federation, Princeton, NJ, pp. 4.199-4.208, October 1995.
- Liu, Y., Iacocca, R.G. and German, R.M., "A challenge to liquid Phase sintering concepts." *Advances in Powder Metallurgy and Particulate Materials*, vol. 1, Metal Powder Industries Federation, Princeton, NJ, pp. 4.199-4.208, October 1995.
- Liu, Y., Iacocca, R., Johnson, J.L., German, R.M., and Kohara, S., Microstructural anomalies in a W-Ni alloy liquid phase sintered under microgravity conditions. *Metallurgical and Materials Transactions*, vol. 26A, pp. 2485-2486 (October 1995).
- Liu, Y., Iacocca, R., Johnson, J.L., German, R.M. and Kohara, S., Microstructural anomalies in a W-Ni alloy liquid phase sintered under microgravity conditions. *Metallurgical and Materials Transactions*, vol. 26A, pp. 2485-2486 (October 1995).
- Lum, J.W., Matson, D.M., and Flemings, M.C. High-speed imaging and analysis of the solidification of undercooled nickel melts. *Met. Trans. B*, vol. 27B, 865 (1996).
- M.E. Glicksman, M.E., "The isothermal dendritic growth experiment on the space shuttle Columbia, The Japan Institute of Metals." *International Symposium on Advanced Materials & Technology for the 21st Century*, Honolulu, Hawaii, December, 1995.
- M.E. Glicksman, M.E., "The isothermal dendritic growth experiment: space flight results from USMP-2 (1994), and USMP-3 (1996)." *Lecture 2, 1996 Summer School on Pattern Formation, Interfacial Dynamics, and Crystal Growth*, Toledo, Spain, May, 1996.
- Matisak, B.P., Zhao, A.X., Narayanan, R., and Fripp, A. The microgravity environment: Its prediction, measurement, and importance to materials processing. *Journal of Crystal Growth*, accepted, (1996).
- Matisak, B.P., Zhao, A.X., Narayanan, R., and Fripp, A. "The microgravity environment: Its prediction, measurement, and importance to materials processing." Presented at The Tenth American Conference on Crystal Growth, August 4-9, 1996, Vail, CO.
- Matisak, B.P., Zhao, A.X., Narayanan, R., and Fripp, A. Experimental verification of agreement between thermal and real-time visual melt-solid interface positions in vertical Bridgman grown Germanium. *J. Crystal Growth*, vol 160, 55-58 (1996).
- Matson, D.M., Shokuhfar, A., Lum, J.W., and Flemings, M.C. "Imaging the double recalescence behavior of Fe-Cr-Ni steel alloys." *Solidification Science and Processing* (I. Ohnaka and D.M. Stefanescu, eds.), TMS Warrendale, Pennsylvania, p 19 (1996).
- Mazuruk, K., Sha, Y.-G., Su, C.-H., and Lehoczy, S.L. Viscosity of $Hg_{0.84}Zn_{0.16}Te$ Pseudobinary Melt. *J. Appl. Physics*, vol. 79(12), 9080-9083 (1996).

Moosbrugger, J.C. Continuum Slip Viscoplasticity with the Haasen Constitutive Model: Application to CdTe Single Crystal Inelasticity. *International Journal of Plasticity*, vol. 11, 799 - 826 (1995).

Moosbrugger, J.C., and Levy, A. Constitutive Modeling for CdTe Single Crystals. *Metallurgical and Materials Transactions A*, vol. 26A, 2687-2697 (1995).

Moosbrugger, J.C., Horton, M.R., and Stevens, T.E. "Inelastic Slip-Dislocation Density Constitutive Model for CdTe Single Crystals." *Computational Mechanics '95*, S.N. Athuri, G. Yagawa, and T.A. Cruse, Eds., vol. 1, Springer, New York, pp 562-57, 1995.

Morton, C.W., Hofmeister, W.H., and Bayuzick, R.J. "The Statistical Analysis of Undercooling Data." *Naval Research Laboratory*, Washington, D.C., September 1996.

Ostrogorsky, A.G. "Space- and Ground-Based Crystal Growth Using a Magnetically Coupled Baffle." *Microgravity Materials Science Conference*, Von Braun Civic Center, Huntsville, Alabama, June 10-11, 1996, pp 138-139.

Raghothamachar, B., Chung, H., Dudley, M., and Larson, Jr., D.J. "Studies on the Influence of Post-Solidification Cooling Rate on the Crystalline Perfection of CdZnTe Single Crystals by Synchrotron White Beam X-ray Topography." *National Synchrotron Light Source Activity Report 1995*, E.Z. Rothman, ed., BNL, Associated University, Inc., 1996.

Raghothamachar, B., Chung, H., Dudley, M., and Larson, Jr., D.J. "Surface Topography Studies of an As-Grown Boule of CdZnTe." *National Synchrotron Light Source Activity Report 1995*, E.Z. Rothman, ed., BNL, Associated University, Inc., 1996.

Raghothamachar, B., Chung, H., Dudley, M., and Larson, Jr., D.J. "Synchrotron X-Ray Topographic Studies on the Causes and Nature of Twinning in CdZnTe Crystals." *National Synchrotron Light Source Activity Report 1995*, E.Z. Rothman, ed., BNL, Associated University, Inc., 1996.

Raghothamachar, B., Chung, H., Dudley, M., and Larson, Jr., D.J. "Synchrotron X-ray Topography Studies on the Formation of Slip Bands and Subgrain Boundaries in Bridgman-Grown CdZnTe Single Crystals." *National Synchrotron Light Source Activity Report 1995*, E.Z. Rothman, ed., BNL, Associated University, Inc., 1996.

Rogers, M.J.B., Matisak, B.P., and Alexander, J.I.D. Venting force contributions to accelerations on USML-1. *Microgravity Science and Technology*, vol. VII/4, 293-297 (1995).

Rosch, W.R., Fripp, A.L., Debnam, W.J., and Pendergrass, T.K. "Vertical Bridgman research Part 1: Performance testing of a vertical Bridgman furnace." Presented at The Tenth American Conference on Crystal Growth, August 4-9, 1996, Vail, CO.

Rosch, W.R., Fripp, A.L., Debnam, W.J., and Pendergrass, T.K. "Vertical Bridgman research Part 2: Verification of a vertical Bridgman numerical model." Presented at The Tenth American Conference on Crystal Growth, August 4-9, 1996, Vail, CO.

Rosch, W.R., Fripp, A.L., Debnam, W.J., and Pendergrass, T.K. "Vertical Bridgman research Part 3: Extension of experimental measurements and numerical modeling." Presented at The Tenth American Conference on Crystal Growth, August 4-9, 1996, Vail, CO.

Rosch, W.R., Fripp, A.L., Debnam, W.J., and Pendergrass, T.K. Performance testing of a vertical Bridgman furnace using experiments and numerical modeling. *Journal of Crystal Growth*, accepted, (1996).

Rulison, A., Rhim, W.K., Morton, C.W., Hofmeister, W.H., and Bayuzick, R.J. Liquid to Solid Nucleation in Two Representative Grades of Commercially Available Zirconium. *NASA Tech Brief*, NPO-19727, (1996).

Schiffman, R.A., "Development of a university based remote teleoperations site for the performance of experiments in microgravity." *8th International Symposium on Experimental Methods for Microgravity Materials Science*, (The TMS, Warrendale, PA, in press 1996).

Sen, S., Dhindaw, B.K., Stefanescu, D.M., Catalina, A., and Curreri, P.A. Melt convection effects on the critical velocity of particle engulfment. *J. of Crystal Growth*, (accepted, 1996).

Seyan, I., Ratke, I., Bender, W., and Voorhees, P.W., Ostwald ripening of solid-liquid Pb-Sn dispersions. *Metall. Trans. A*, (1996).

Sha, Y.-G., Su, C.-H., Alexander, H.A., Lehoczky, S.L., and Wang, J.-C. Seeded Growth of HgTe-ZnTe by Directional Solidification Using an Initial Composition Profile Simulating a "Diffusion-Boundary" Layer. *J. Crys. Growth* (in press, 1996).

Sha, Y.-G., Su, C.-H., and Lehoczky, S.L. "Mass Flux of ZnSeS and ZnSeTe by Physical Vapor Transport." MRS Fall Meeting, Boston, Massachusetts, November 27 - December 1, 1995.

Sha, Y.-G., Su, C.-H., and Lehoczky, S.L. Growth of HgTe-ZnTe by Directional Solidification in a Magnetic Field. *J. Crys. Growth* (in press, 1996).

Sha, Y.-G., Su, C.-H., and Lehoczky, S.L. Intrinsic Carrier Concentrations and Electron Effective Masses in $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$. *J. Appl. Physics* (in press, 1996).

Sha, Y.-G., Su, C.-H., and Lehoczky, S.L. "Seeded Growth of HgTe-ZnTe by Directional Solidification using Initial Composition Profile Simulating a "Diffusion-Boundary" Layer." The 10th American Conference on Crystal Growth, Vail, Colorado, August 4-9, 1996.

Sha, Y.-G., Su, C.-H., Lehoczky, S.L., and Szofran, F.R. "Ground-Based growth of HgTe-ZnTe in a Magnetic Field." Proceedings of the 34th Aerospace Sciences Meeting and Exhibit, Reno, Nevada, January 15-18, 1996 (paper AIAA 96-0256).

Sha, Y.-G., Su, C.-H., Mazuruk, K., and Lehoczky, S.L. Thermal Diffusivity and Conductivity of HgTe-ZnTe Solids and Melts. *J. Appl. Physics*, vol. 80(2), 752-755 (1996).

Sha, Y.-G., Su, C.-H., Mazuruk, K., and Lehoczky, S.L. Phase Diagram, Density, Heat Capacity and Enthalpy of Mixing Pseudobinary $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$ Melts. *J. Appl. Physics*, vol. 80(1), 137-142 (1996).

Stefanescu, D.M. "Particle Pushing and Engulfment by Solidifying Interfaces." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Stevens, T.E., Moosbrugger, J.C., and Carlson, F.M. "High Temperature Deformation Behavior of CdTe (poster presentation)." IUCR Meeting, Seattle, Washington, August 10-17, 1996.

Stevens, T.E., Moosbrugger, J.C., and Carlson, F.M. "High Temperature Deformation Behavior of CdTe (poster presentation)." IUCR Meeting, Seattle, Washington, August 10-17, 1996.

Su, C.-H. "Crystal Growth of ZnSe and Related Ternary Compound Semiconductors by Vapor Transport." Microgravity Materials Science Conference, p 176 conference summaries volume, Huntsville, Alabama, June 10-11, 1996.

Su, C.-H., and Sha, Y.-G. "Current Topics in Crystal Growth Research ("Growth of Wide Band Gap II-VI Compound Semiconductors by Physical Vapor Transport")." Edited by the Council of Scientific Information, Research Trends, vol. 2, pp 401-433, 1995.

Su, C.-H., Gillies, D.C., Szofran, F.R., Watring, D.A., and Lehoczky, S.L. "The Influence of Reduced Gravity on the Crystal Growth of Electronic Materials." Proceeding of the 6th International Space Conference of Pacific Basin Societies (6th ISCOPS), Marina del Ray, California, "Strengthening Cooperation in the 21st Century, Volume 91, Advances in the

Su, C.-H., Gillies, D.C., Szofran, F.R., Watring, D.A., and Lehoczky, S.L. "The Influence of Reduced Gravity on the Crystal Growth of Electronic Materials." Invited paper presented at the 6th International Space Conference of Pacific Basin Societies (6th ISCOPS), Marina del Ray, California, December 6 - 8, 1995.

Su, C.-H., Gillies, D.C., Szofran, F.R., Watring, D.A., and Lehoczky, S.L. "The Influence of Reduced Gravity on the Crystal Growth of Electronic Materials ("Cooperation in the 21st Century: Advances in Astronautical Sciences")." Proceedings of the 6th International Space Conference of Pacific Basin Societies (6th ISCOPS), P.M. Bainum, G.L. May,

Trivedi, R., Tewari, S., and Kurtze, D. "Interface Pattern Selection Criterion for Cellular Structures in Directional Solidification." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

Volz, M.P., Szofran, F.R., Watring, D.A., Gillies, D.C., Su, C.-H., and Lehoczky, S.L. "Magnetic Damping of Convective Flows During Semiconductor Crystal Growth." Proceedings of the International Workshop on High Magnetic Fields, Tallahassee, Florida, February 28 - March 1, 1996 (in press).

Voorhees, P.W., "Coarsening in solid-liquid mixtures." Proceedings of the Microgravity Materials Science Conference, 1996.

Watring, D.A., and Lehoczky, S.L. Magneto Hydrodynamic Damping of Convection during Vertical Bridgman-Stockbarger Growth of HgCdTe. *J. Cryst. Growth*, vol. 164, 478-487 (1996).

Watring, D.A., Lehoczky, S.L., Szofran, F.R., and Gillies, D.C. "Convection Influence on Radial Segregation During Unidirectional Solidification of the Binary Alloy, HgCdTe." Proceedings of SPIE - The International Society for Optical Engineering - 1996 International Symposium on Space Processing of Materials, Denver, Colorado, August 4-6, 1996, vol.

Wiedemeier, H., and Ge, Y.R. Transient Behavior of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ Films Deposited on (100) CdTe Substrates by Chemical Vapor Transport. *J. Electronic Materials*, vol. 25, 1072-1081 (1996).

Wiedemeier, H., and Ge, Y.R. "Transient Behavior of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ Films Deposited on (100) CdTe Substrates by Chemical Vapor Transport." Tenth American Conference on Crystal Growth, Vail, Colorado, August 1996.

Wiedemeier, H., and Hutchins, M.A. The Temperature-Composition Phase Diagram of the HgTe-HgI₂ Pseudobinary System on the HgTe Rich Side. *Z. anorg. allg. Chem.*, vol. 622, 157-163 (1996).

Wiedemeier, H., Ge, Y.R., and Hutchins, M.A. "Vapor Growth of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ Epitaxial Films under Normal and Microgravity Conditions." SPIE Annual Meeting, Symposium Space Processing of Materials, Denver, Colorado, August 1996.

Wunderlich, R.K., Lee, D.S., Johnson, W.L., and Fecht, H.J. Non Contact Modulation Calorimetry of Metallic Liquids in Low Earth Orbit. *Phys. Rev. B, Rapid Commun.* (1996).

Yao, M.W., Matthiesen, D.H., and Chait, A. Numerical simulation of heat transport and fluid flow in directional crystal growth of GaAs. Numerical heat Transfer, Part A: Applications, (accepted, 1996).

Ground: Biotechnology

Akins, R.E., Schroedl, N.A., Gonda, S.R., and Hartzell, C.R. Neonatal rat heart cells cultured in simulated microgravity. *In Vitro Cellular and Developmental Biology*, (In Press).

Ansari, R., Suh, K., Arabshahi, A., Wilson, W., Bray, T., and DeLucas, L. "A Fiber Optic Probe for Monitoring Protein Aggregation, Nucleation and Crystallization." Sixth International Conference on Crystallization of Biological Macromolecules, Hiroshima, Japan, November 1995.

Arabshahi, A., and Wilson, W. "Automated Dynamic Control of Protein Crystal Growth Utilizing Temperature and Laser Light Scattering." 47th Southeast 151st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, Tennessee, November 1995.

Arango, H., Satyaswaroop, P., Cavanagh, D., Goldrain, V., and Becker, J. Effects of 17 beta-estradiol and mifepristone (RU486) on Ishikawa human endometrial cancer cell line. *Am. Assoc. Cancer Res.*, No. 2231, (1996).

Arango, H., Satyaswaroop, P., Cavanaugh, D., and Becker, J. The growth inhibitory effects of onapristone (ZK98299) and mifepristone (RU486) on Ishikawa human endometrial cancer cell line. *West. Assoc. Gynecol. Oncol.*, (1996).

Arnold, M. "Optical sensor designs for remote, selective, reliable, and continuous monitoring." First Gordon Conference on Chemical Sensors and Interfacial Design, Colby-Sawyer College, New London, New Hampshire, July 28, 1996.

Arnold, M., Murhammer, D., and Cohen, M. "Continuous, non-invasive monitoring of rotating wall vessels and applications to the study of prostate cancer." Investigators' Working Group Meeting, Microgravity Sciences and Applications Division, NASA, February 23, 1996.

- Asanov, A., DeLucas, L., Oldham, P., and Wilson, W. "Interfacial Protein Aggregation Related to Crystallization Conditions Studied by Total Internal Reflection Fluorescence." 47th Southeast 151st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, Tennessee, November 1995.
- Baldwin, S.P. and Saltzman, W.M. Polymers for tissue engineering. *Trends in Polymer Science*, 4, 177-182 (1996).
- Baldwin, S.P., Krewson, C.E., and Saltzman, W.M. PC12 cell aggregation and neurite growth in gels of collagen, laminin, and fibronectin. *International Journal of Developmental Neuroscience*, 14, 351-364 (1996).
- Becker, J. "The benefits of space research on women's health." Annual meeting of the Society for Women Engineers, Melbourne FL, 1996.
- Becker, J. "Hormonal modulation of human endometrial carcinoma growth." NASA-JSC Investigatory Working Group, Meeting, 1996.
- Becker, J.L., Papenhausen, P.R., and Widen, R.H. Cytogenetic, morphologic and oncogene analysis of a cell line derived from a heterologous mixed müllerian tumor of the ovary. *In Vitro Cell. Develop. Biol.*, (In Press).
- Bonita, J., Arnold, E., and Wiencek, J.M. "Effect of Crystal Growth Rate on Protein Crystal Quality." AIChE Annual Meeting, Miami Beach, Florida, November 1995.
- Bursac, P.M., Freed, L.E., Biron, R.J., and Vunjak-Novakovic, G. Mass transfer studies of tissue engineered cartilage. *Tissue Engineering*, 2, 141-150 (1996).
- Bursac, P.M., Freed, L.E., Biron, R.J., and Vunjak-Novakovic, G. Mass transfer studies of tissue engineered cartilage. *Tissue Engineering*, 2:141-150 (1996).
- Bursac, P., Vunjak-Novakovic, G., Biron, R., and Freed, L.E. "Mass Transfer Studies of Tissue Engineered Cartilage." Annual meeting of the BMES, Boston MA. October, 1995, 23:S-52.
- Bursac, P., Vunjak-Novakovic, G., Biron, R., and Freed, L.E. "Mass Transfer Studies of Tissue Engineered Cartilage." Annual Meeting of the BMES, Boston MA, October 1995. 23: S-52.
- Campbell-Washington, J., Craig, J.N., Baker, T., Risin, D., Goodwin, T.J., and Pellis, N.R. "Differential display RT-PCR analysis and cloning of novel mRNAs expressed in HL-60 promyelocytic cells cultured in simulated microgravity conditions." ASBMB/ASIP/AII Joint Meeting, New Orleans, Louisiana, June 6-8, 1996.
- Campbell-Washington, J., Craig, J.N., Baker, T., Risin, D., Goodwin, T.J., and Pellis, N.R. Differential display RT-PCR analysis and cloning of novel mRNAs expressed in HL-60 promyelocytic cells cultured in simulated microgravity conditions. *FASEB J.*, 10(6), (Abst.) (April 30, 1996).
- Cape, S.P., Lee, C.-Y., Petrini, K., Ferree, S., Sportiello, M.G., and Todd, P. "Chromatographic purification of oligonucleotides: comparison with electrophoresis." Colorado Biotechnology Symposium, Ft. Collins, Colorado, 1996.
- Cape, S.P., Lee, C.-Y., Petrini, K., Ferree, S., Sportiello, M.G., and Todd, P. "Chromatographic purification of oligonucleotides: comparison with electrophoresis." Biochemical Engineering Symposium, Manhattan, Kansas, 1996.
- Carter, Jr., C.W. A Local Approximation to Supersaturation Affords a Useful Coordinate Transformation for the Study of Crystal Growth. *Acta Crystallographica*, vol. D52, 647-654 (1996).
- Cassanto, J.M., Morrison, D.R., Hymer, W., Todd, P., Korszun, Z.R., Mosier, B., Edmundson, A., Sygusch, J., Bower, D., Kearney, G.P., Dunfee, W., Alvarado, U., Guintini, R., and Bem, M. "Concept of a commercial automated biotechnology space processing payload onboard the space shuttle and space station." *Proceedings of the Space Technology &*
- Chung, H. and Arnold, M. "Development of an optical oxygen sensor with a radioluminescent light source." Pittcon'96, Chicago, IL, March 7, 1996.
- Chung, H., Arnold, M., Rhiel, M., and Murhammer, D. Simultaneous measurements of glucose, glutamine, ammonia, lactate, and glutamate in aqueous solutions by near-infrared spectroscopy. *Applied Spectroscopy*, 50, 270-276 (1996).

- Chung, S.K., and Trinh, E.H. "An ultrasonic-electrostatic hybrid levitator for crystal growth from solution." Joint Acoustical Societies of America and of Japan (abstract accepted), December 2-6, 1996.
- Clejan, S., O'Connor, K.C., Cowger, N.L., Cheles, M.K., Haque, S., and Primavera, A.C. Effects of simulated microgravity on DU 145 human prostate carcinoma cells. *Biotechnol. Bioeng.*, 50, 587-597 (1996).
- Cohen, M., Griebing, T., Aherghotu, C.A., Rokhlin, O., and Ross, J. Cellular adhesion molecules in urologic malignancies. *American Journal of Clinical Pathology*, (In Press).
- Cooney, C. and Towe, B.C. Carbon Dioxide Measurement by Microflow Colorimeter. *Journal of Biosensors and Bioelectronics*, (In Press).
- Cooper, D. and Pellis, N.R. "Cell-cell and cell-matrix interactions aid mitogen induced T lymphocyte activation in simulated microgravity." ASBMB/ASIP/AII Joint Meeting, New Orleans, Louisiana, June 6-8, 1996.
- Cooper, D. and Pellis N.R. Cell-cell and cell-matrix interactions aid mitogen induced T lymphocyte activation in simulated microgravity. *FASEB J.*, 10(6), (Abst.) (April 30, 1996).
- Cowger, N.L., O'Connor, K.C., and Bivins, J.E. Influence of simulated microgravity on the longevity of insect-cell culture. *Enzyme Microb. Technol.*, In press, (1996).
- Cowger, N.L., O'Connor, K.C., and Bivins, J.E. Characterization of microgravity cultures of insect cells in stationary and death phase. *In Vitro Cell. Dev. Biol.*, 32, 37A (1996).
- Cowger, N., O'Connor, K., and Bivins, J. "Characterization of microgravity cultures of insect cells in stationary and death phase." 1996 World Congress on In Vitro Biology: Society for In Vitro Biology, San Francisco, CA, 1996.
- Cowger, N., O'Connor, K., and Bivins, J. "Behavior of insect cells during long-term cultivation in simulated microgravity." Annual Meeting of the American Institute of Chemical Engineers, Chicago, IL, 1996.
- Dai, W. and Saltzman, W.M. Fibroblast aggregation by suspension with conjugates of poly(ethylene glycol) and RGD. *Biotechnology and Bioengineering*, 50, 349-356 (1996).
- Darcy, P.A., and Wiencek, J.M. "Thermal Analysis of Protein Crystallization." Symposia on Protein Crystallization, American Chemical Society Meeting, New Orleans, Louisiana, March 24, 1996.
- DeTitta, G.T. "Preliminary Evaluation of Thermal Gradients as Tools for Macromolecular Crystal Growth." Recent Advances in Macromolecular Crystallization, LeBiscenbourg, France, June 2-4, 1996.
- DeTitta, G.T. "HOT and COLD: The Story of Three Thermal Gradients in Search of the Perfect Crystal." Protein Crystal Growth Conference, Panama City Beach, Florida, April 28-30, 1996.
- DeTitta, G.T., Dembik, D.M., Pangborn, W.A., and Luft, J.R. "Polythermal Screening and Production Methods for Macromolecular Crystallization." International Union of Crystallography XVII Congress and General Assembly, Seattle, Washington, August 8-17, 1996.
- DeYoreo, J.J., Land, T.A., Malkin, A.J., Kuznetsov, Yu.-G., Lee, J.D., and McPherson, A. "In situ AFM investigation of step dynamics and surface morphological evolution during growth from solutions." Dynamics of Crystal Surfaces and Interfaces, Traverse City, MI, August 1996.
- DeYoreo, J.J., Malkin, A.J., Land, T.A., Kuznetsov, Yu.-G., Lee, J.D., and McPherson, A. "An AFM study of growth mechanisms and morphologies of solution based crystals." TMS annual meeting, Anaheim, CA, February 1996.
- DISSERTATION Zhou, X. to Murhammer, D. "Near infrared spectroscopy for monitoring bioreactor components and chemiluminescence sensors for hydrogen peroxide, glucose, and nitric oxide, Ph. D. Thesis, University of Iowa, Iowa City, IA." 1996.
- Ducheyne, P. "The Use of Bioactive Glass Particles as Microcarriers in Microgravity Environment." Biotechnology Program, Investigators Working Group meeting, Houston, Texas, February 1996.

Ducheyne, P., Gao, H., El-Ghannam, A., Shapiro, I., and Ayyaswamy, P. "The use of bioactive glass particles as microcarriers." International Mechanical Engineering and Exposition, Atlanta, GA 1996.

Ducheyne, P., Schepers, E., and Shapiro, I. Bone bioactive material surface changes and bone cell function are related. *Bioceramics 9*, Ed. T. Kokubo, Elsevier, Oxford, England, (1996).

Durzan, D. "Taxane biosynthesis at the individual cell level." VivoRx Pharmaceuticals, April 23, 1996.

Patent Approved, U.S. Patent #: 5,547,866

Durzan, D. and Ventimiglia, F. "Taxane production in haploid derived cell cultures."

Durzan, D., Ventimiglia, F., Falk, R., and Havel, L. "Covalently bound taxanes in yeast suspension cultures ." *Cellular and Molecular Biology 42/Congress Suppl.*: 27. Abst. 34, 1996.

El-Ghannam, A., Ducheyne, P., and Shapiro, I. Porous bioactive glass and hydroxyapatite stimulate bone cell function in vitro along different time lines. *J. Biomed. Mater. Research*, (In Press).

Emoto, K., Harris, J.M., and Van Alstine, J.M. "Electrokinetic evaluation of polymer coatings for use in capillary electrophoresis." *Electrophoresis Society Meeting*, Atlanta, Georgia, May 1996.

Emoto, K., Harris, J.M., and Van Alstine, J.M. "Improved polymer coatings for use in separation science." 18th International Symposium on Capillary Chromatography Riva Del Garda, Italy, May 20-24, 1996.

Feigelson, R.S., De Mattei, R.C., and DeLucas, L. "Laser Scattering Tomography - a Technique for Studying Crystal Defects, Their Relationship to Growth Conditions and Their Effect on Diffraction." *Protein Crystal Growth*, Panama City Beach, Florida, April 29-30, 1996.

Francis, K. and Palsson, B.O. Effective Communication Distances in Complex Cell Cultures are Determined by the Relative Cytokine Secretion and Diffusion Time Constants. In Preparation, (1996).

Francis, K.M., O'Connor, K.C., and Spaulding, G.F. Cultivation of fall armyworm ovary cells in simulated microgravity. *In Vitro Cell. Dev. Biol.*, In Press, (1996).

Francis, K.M., O'Connor, K.C., Blake, D.A., Caldwell, D.R., and Spaulding, G.F. "Growth and structure of corneal tissue in simulated microgravity." 959-963. *Animal Cell Technology: Developments Towards the 21st Century*, Kluwer Academic Publishers, Dordrecht, 1995.

Freed, L.E. and Vunjak-Novakovic, G. Microgravity tissue engineering. *In Vitro Cell. Dev. Biol.*, (In Press).

Freed, L.E. and Vunjak-Novakovic, G. "Tissue Culture Bioreactors: Chondrogenesis as a Model System," in "Textbook of Tissue Engineering." Edited by: RP Lanza, R. Langer, W. Chick. R.G. Landes Company, Austin, Texas, Chapter 11, pp 150-158, 1996.

Freed, L.E. and Vunjak-Novakovic, G. Microgravity tissue engineering. *In Vitro Cell. Dev. Biol.*, (In Press).

Freed, L.E., Vunjak-Novakovic, G. "Tissue culture bioreactors: chondrogenesis as model system," in "Textbook of Tissue Engineering." Edited by: RP Lanza, R. Langer, W. Chick. R.G. Landes Company, Austin, Texas, Chapter 11, pp 150-158, 1996.

Frey, W., Schief, Jr., W.R., and Vogel, V. Two-dimensional crystallization of streptavidin studied by quantitative Brewster Angle Microscopy. *Langmuir*, vol. 12, 1312-1320 (1996).

Frey, W., Schief, Jr., W.R., Pack, D., Chen, C.-T., Chilcote, A., Stayton, P.S., Vogel, V., and Arnold, F.H. 2-D protein crystallization via metal-ion coordination by naturally-occurring surface histidines. *Proc. Natl. Acad. Sciences USA*, vol. 93, 4937-4941 (1996).

Gallagher, T., Oliver, J., Bott, R., Betzel, C., and Gilliland, G.L. The structure of subtilisin BPN' at 1.6Å resolution and three high-resolution crystal forms compared. *Acta Crystallographica D*, (accepted for publication 5/96).

- Galvan, D.L., Hayman, G.T., Goodwin, T.J., Chatman, D.Y., Unsworth, B.R., and Lelkes P.I. "Simulated microgravity induces neuroendocrine differentiation of PC12 pheochromocytoma cells." 1996 World Congress on In Vitro Biology, San Francisco, CA, June 22-27, 1996.
- Galvan, D.L., Lelkes, P.I., Wankowski, D.M., Goodwin, T.J., and Unsworth, B.R. "Simulated microgravity conditions enhance neuroendocrine organoid formation in vitro." Aviation and Space Medicine Association, 67th Annual Scientific Meeting, Atlanta, GA, May 5-9, 1996.
- Galvan, D.L., Liu, J., Wankowski, D.M., Lelkes, P.I., and Unsworth B.R. "Differential modulation of extracellular matrix protein expression in adrenal medullary cells cultured under simulated microgravity conditions." Mol. Biol. Cell, Nov. 6S:975. 1995.
- Gernert, K.M., Thomas, B.D., Plurad, J.C., Richardson, J.S., Richardson, D.C., and Bergman, L.D. "Puzzle Pieces Defined: Locating Common Packing Units in Tertiary Protein Contacts." Proceedings of Pacific Symposium on Biocomputing. January 1996.
- Gooch, K.J., Langer, R., Freed, L.E., and Vunjak, G. "In Vitro Vasculogenesis." Annual Meeting of the BMES. University Park, PA. October, 1996.
- Goodwin, T.J., Canales, D.D., and Baker, T.L. "Three-dimensional tumor modeling for use in lymphokine-activated killer cell invasion.." 1996 world Congress on In Vitro biology, San Francisco, California, June 22-27, 1996.
- Goodwin, T.J., Prewett, T.L., Spaulding, G.F., and Becker, J.L. Three-dimensional culture of a mixed mullerian tumor of the ovary: expression in vivo characteristics. In Vitro Cell Develop. Biol., (In Press).
- Guo, B., and Wilson, W. "Static and Dynamic Solution Properties of the Protein Ovostatin as Determined by Laser Light Scattering." 47th Southeast 151st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, Tennessee, November 1995.
- Hammond, T.G., Majewski, R.R., Galvan, D.L., and Lelkes, P.I. De novo expression of aminoglycoside and myeloma protein receptors in renal proximal tubular cells grown in simulated microgravity: a new model for pharmacological protection studies. In Vitro Cell & Dev Biol, 32:44A, (1996).
- Hammond, T.G., Majewski, R.R., Kaysen, J.H., Goda, F.O., Navar, G.L., Pontillon, F., and Verroust P.J. Gentamicin Inhibits Rat Renal Cortical Homotypic Endosomal Fusion: Role of megalin. Am J Physiol, (In Press).
- Hammond, T.G., Majewski, R.R., Pontillon, F., Verroust, P.J., Goodwin, T.J., Paddock, S.W., Galvan, D.L. and Lelkes, P.I. H+ATPase dependence of "degradative pathway" endosomal fusion. (Submitted).
- Havel, L. and Durzan, D. Apoptosis in plants. Botanica Acta, 109, 268-277 (1996).
- Havel, L. and Durzan, D. Apoptosis during diploid parthenogenesis and early somatic embryogenesis of Norway Spruce. Intl. J Plant Science, 157, 8-16 (1996).
- Hillhouse, T., Arabshahi, A., and Wilson, W. "Using Temperature to Grow Protein Crystals." 16th Annual Undergraduate Chemistry Research Conference, Memphis, Tennessee, March 1996.
- Ho, M.L., Molnar, G., Funanage, V.L., and Schroedl, N.A. Myogenic factor expression and quantitation in satellite cells derived from growth rat muscle. BAM, 6(3), 145-155 (1996).
- Hughes, J.H., Pierson, S., and Long, J.P. "The Effects of Microgravity on Viral Replication." NASA Biotechnology Conference, Houston, TX., February 23-24, 1996.
- Ingram, M., Techy, G.B., Saroufeem, R., Yazan, O., Narayan, K.S., Goodwin, T., and Spaulding, G.F. Three-dimensional growth patterns of various human tumor cell lines in simulated microgravity of a NASA bioreactor. In Vitro J. Soc., In Vitro Biol., In Press, (1996).
- Inouye, H., and Kirschner, D.A. "Intersheet hydrophobic cores in fibrillar amyloid assembled from Alzheimer's disease A-beta and scrapie PrP peptides." 27th annual meeting of the American Society for Neurochemistry, Philadelphia, Pennsylvania, March 1996.

- Inouye, H., and Kirschner, D.A. "Refined fibril structures: The hydrophobic core in Alzheimer's beta-amyloid and prion as revealed by X-ray diffraction." *The Nature and Origin of Amyloid Fibrils*, CIBA Foundation Symposium No. 199, pp 22-39, John Wiley & Sons, Chichester, United Kingdom and New York, New York (1996).
- Jessup, J.M., Brown, D., Fitzgerald, W., Ford, R.D., Nachman, A., Goodwin, T.J., and Spaulding, G. Induction of Carcinoembryonic Antigen Expression in a Three-Dimensional Culture System. *In Vitro Cell Biol Develop.*, (In Press).
- Jessup, J.M., Goodwin, T.J., Garcia, R., and Pellis, N.R. "STS-70: Flight of EDU-1." *NASA Symposium: Cell Culture Bioreactor and Three-Dimensional Culture Studies*, World Congress on In Vitro Biology, San Francisco, California, June 25, 1996.
- Johnson, T., Todd, P., and Stodieck, L. "Microgravity: New opportunities to facilitate biotechnology development." *Proceedings of the Space Technology & Applications International Forum*, Albuquerque, New Mexico, Institute for Space Power, University of New Mexico, paper #275, 1996.
- Kim, B.S. and Palsson, B.O. Clinical Scale Production of Human Hematopoietic Progenitors in a Suspense Bioreactor. Submitted, (1996).
- Kirschner, D.A. "Refined Fibril Structures." *CIBA Foundation Symposium on "e Nature and Origin of Amyloid Fibrils*, Oeiras, Portugal.
- Kirschner, D.A. "Amyloid Fibril Structures." *CIBA Foundation/Calouste Gulbenkian Foundation, Open Meeting on The Nature and Origin of Amyloid Fibrils*, Lisbon, Portugal.
- Kirschner, D.A. "Fibrilogenesis in Alzheimer's disease." *University of Virginia*, April 1996.
- Kirschner, D.A. "Trials and tribulations in fabricating oriented amyloid fibrils for x-ray diffraction." *Protein Crystal Growth Conference*, April 1996, Microgravity Materials Science Conference.
- Kirschner, D.A. "Targeting fibrilogenesis in Alzheimer's disease." *Pharmaceutical Peptides, Inc.*, Cambridge, Massachusetts, May 1996.
- Konnert, J.K. "Atomic Force Microscope Studies of Protein Crystal Growth: (a) Observations at up to 10x Supersaturation, (b) Modeling and Interpretation of Observed Molecular Features." *Protein Crystal Growth Conference*, Panama City, Florida, April 28-30, 1996.
- Krewson, C.E. and Saltzman, W.M. Nerve growth factor delivery and cell aggregation enhance choline acetyltransferase activity after neural transplantation. *Tissue Engineering*, 2, 183-196 (1996).
- Kuznetsov, Yu.-G., Malkin, A.J., and McPherson, A. "Interferometric studies of macromolecular crystal growth." *Proceedings of the 6th International conference on crystallization of biological molecules*, 58 (1995).
- Kuznetsov, Yu.-G., Malkin, A.J., and McPherson, A. "Defect structure of protein and virus crystals studied by in situ atomic force microscopy." *Proceedings of the 10th American conference on crystal growth*, 37 (1996).
- Land, T.A., DeYoreo, J.J., Malkin, A.J., Kuznetsov, Yu.-G., McPherson, A., and Lee, J.D. "An in situ atomic force microscopy study of canavalin crystal growth." *Proceedings of the 10th American conference on crystal growth*, 12 (1996).
- Land, T.A., DeYoreo, J.J., Malkin, A.J., Kuznetsov, Yu.-G., McPherson, A., and Lee, J.D. "An in situ atomic force microscopy study of canavalin crystal growth." *Protein Crystal Growth*, Panama City, Florida, April 1996.
- Land, T.A., Malkin, A.J., Kuznetsov, Yu.-G., DeYoreo, J.J., and McPherson, A. "Investigation of canavalin crystallization using in situ atomic force microscopy." *Proceedings of the 6th International conference on crystallization of biological molecules*, 77 (1996).
- Land, T.A., Malkin, A.J., Kuznetsov, Yu.-G., McPherson, A., and DeYoreo, J.J. Mechanisms of protein crystal growth: An atomic force microscopy study of canavalin crystallization. *Physical Review Letters*, vol. 75, no. 14, 2774-2777 (1995).

Lee, C.-Y., and Todd, P. "Characterization and application of osmotic dewatering to the crystallization of biomolecules." American Chemical Society Annual National Meeting, New Orleans, Louisiana, March 24-28, 1996.

Lee, C.Y., Sportiello, M.G., Cape, S., Ferree, S., Todd, P., Kundrot, C.E., and Barnes, C. "Application of osmotic dewatering to the crystallization of oligonucleotides for crystallography." Proceedings of 25th Biochemical Engineering Symposium, R. Bajpai, ed., University of Missouri, Columbia, Missouri, 1995.

Lee, C.-Y., Sportiello, M.G., Cape, S.P., Ferree, S., Todd, P., Kundrot, C.E., Lietzke, S., and Barnes, C. "Characterization and application of osmotic dewatering to the crystallization of oligonucleotides." Colorado Biotechnology Symposium, Ft. Collins, Colorado, 1996.

Lee, C.-Y., Sportiello, M.G., Cape, S.P., Ferree, S., Todd, P., Kundrot, C.E., Lietzke, S., and Barnes, C. "Characterization and application of osmotic dewatering to the crystallization of oligonucleotides." Biochemical Engineering Symposium, Manhattan, Kansas, 1996.

Lelkes, P.I., Galvan, D.L., Hayman, G.T., Goodwin, T.J. Chatman, D.Y., Cherian, S., Garcia R.M.G., and Unsworth B.R. Simulated microgravity conditions enhance differentiation of cultured PC12 cells towards the neuroendocrine phenotype. In Vitro Cell and Developmental Biology, Animal, (Submitted).

Lietzke, S.E., Barnes, C.L., Berglund, J.A., and Kundrot, C.E. The structure of an RNA dodecamer shows how tandem U-U base pairs increase the range of stable RNA structures and the diversity of recognition sites. Structure, vol. 4, 917-930 (1996).

Lin, H., Vekilov, P.G., and Rosenberger, F. Facet morphology response to nonuniformities in nutrient and impurity supply. II. Numerical modeling. J. Crystal Growth, vol. 158, 552-559 (1996).

Luft, J.R., Albright, D.T., Baird, J.K., and DeTitta, G.T. The Rate of Water Equilibration in Vapor-Diffusion Crystallizations: Dependence on the Distance from the Droplet to the Reservoir. Acta Crystallographica, vol. D52, 1098-1106 (1996).

Mahoney, M.J. and Saltzman, W.M. Controlled release of proteins to tissue transplants for the treatment of neurodegenerative disorders. Journal of Pharmaceutical Science, (In Press).

Malkin, A.J., Kuznetsov, Yu.-G., and McPherson, A. Incorporation of microcrystals by growing protein and virus crystals. Proteins: Structure, Function and Genetics, vol. 24, 247-252 (1996).

Malkin, A.J., Kuznetsov, Yu.-G., and McPherson, A. "Atomic force microscopy studies of macromolecular crystal growth." East Coast Conference on crystal growth, Atlantic City, New Jersey, October 1995.

Malkin, A.J., Kuznetsov, Yu.-G., Glantz, W., and McPherson, A. Atomic force microscopy studies of surface morphology and growth kinetics in thaumatin crystallization. J. Physical Chemistry, vol. 100, 11736-11743 (1996).

Malkin, A.J., Kuznetsov, Yu.-G., Glantz, W., and McPherson, A. "Atomic force microscopy studies of surface morphology and growth kinetics in thaumatin crystallization." Proceedings of the 10th American conference on crystal growth, 34 (1996).

Malkin, A.J., Kuznetsov, Yu.-G., Glantz, W., and McPherson, A. "An in situ atomic force microscopy study of thaumatin crystal growth." Protein Crystal Growth, Panama City, Florida, April 1996.

Malkin, A.J., Kuznetsov, Yu.-G., Land, T.A., DeYoreo, J.J., and McPherson, A. Mechanisms of growth for protein and virus crystals. Nature Structural Biology, vol. 2, no. 11, 956-959 (1995).

Malkin, A.J., Kuznetsov, Yu.-G., Land, T.A., DeYoreo, J.J., and McPherson, A. "In situ atomic force microscopy studies of protein and virus crystal growth." Proceedings of the 6th International conference on crystallization of biological molecules, 27 (1995).

Malkin, A.J., Land, T.A., Kuznetsov, Yu.-G., McPherson, A., and DeYoreo, J.J. Investigation of virus crystal growth by in situ atomic force microscopy. Physical Review Letters, vol. 75, no. 14, 2778-2881 (1995).

- Malmsten, M., and Van Alstine, J.M. Adsorption of poly(ethylene glycol) amphiphiles to form coatings which inhibit protein adsorption. *J. Colloid Interf. Sci.*, vol. 177, 502-512 (1996).
- Malmsten, M., and Van Alstine, J.M. Adsorption of poly(ethylene glycol) amphiphiles to form coatings which inhibit protein adsorption. *J. Interf. Sci.*, vol. 177, 502-512 (1996).
- Malmsten, M., Lassen, B., Van Alstine, J.M., and Nilsson, U. Adsorption of serum complement proteins C1g and C3. *J. Colloid Interf. Sci.*, vol. 178, 123-134 (1996).
- Martin, A. "Preservation of human thyroid organoids in the scid mouse." International symposium on endocrine cell transplantation and genetic engineering, Giessen, Germany, June 16-19, 1996 (Official satellite meeting of the 10th International Congress of the Endocrinology, Invited Presentation).
- Martin, A., Matsuoka, N., Concepcion, E., and Davies T. F. Endogenous antigen presentation by autoantigen-transfected Epstein-Barr Virus lymphoblastoid cells: T-cell receptor N-region hydrophobicity relates to thyroid antigen recognition. *Autoimmunity*, 21:223-230 (1995).
- Martin, A., Zhang, J., Unger, P., and Shultz L. D. "T-cell-receptor V gene selection in human thyroid organoids." *Thyroid* 5 (Supplement 1): 392, 11th International Thyroid Congress, Toronto, Canada, September 10-15, 1995.
- Martin, A., Zhou, A., Unger, P., Katz, N., Gordon, R., and Davies T.F. "Thyroid cell growth under low-shear conditions: Three-dimensional organization of SV40 transformed thyroid cells." 10th International Congress of Endocrinology, June 12-15, 1996.
- McPherson, A., Malkin, A.J., and Kuznetsov, Yu.-G. "Defect structure of macromolecular crystals." *Protein Crystal Growth*, Panama City, Florida, April 1996.
- McPherson, A., Malkin, A.J., Kuznetsov, Yu.-G., and Koszelak, S. "Incorporation of impurities into macromolecular crystals." *Proceedings of the 6th International conference on crystallization of biological molecules*, 108 (1995).
- Molnar, G., Ho, M.L., and Schroedl, N.A. Evidence for multiple satellite cell populations and a nonmyogenic cell type that is regulated differently in regenerating and growing skeletal muscle. *Tissue and Cell*, (In Press).
- Molnar, G., Ho, M.L., and Schroedl, N.A. RMo myoblasts express a mature skeletal muscle phenotype in the absence of the intermediate filament protein desmin. *J. Cell. Physiol.*, (Submitted).
- Molnar, G., Schroedl, N.A., Gonda, S.R., and Hartzel, C.R. Skeletal muscle satellite cells cultured in simulated microgravity. *In Vitro Cellular and Developmental Biology*, (In Press).
- Morré, D.J. "tNOX, a new cell surface anticancer drug target (invited presentation)." *NASA/NIH. Structure-Based Design Conference*. Panama City Beach, Florida, April 25-28, 1996.
- Morré, D.J., Chueh, P.-J., Wu, L.-Y., and Morré, D.M. The antitumor sulfonylurea-inhibited NADH oxidase activity of HeLa plasma membrane vesicles has characteristics of a protein disulfide-thiol interchange protein. *Mol. Biol. Cell*, vol. 6, no. 328a, (1995).
- Morré, D.J., Wilkinson, F.E., Kim, C., Cho, N., Lawrence, J., Morré, D.M., and McClure, D. Antitumor sulfonylurea-inhibited NADH oxidase of cultured HeLa cells shed into media. *Biochim. Biophys. Acta*, vol. 1280, 197-206 (1996).
- Morré, D.M., Sammons, D.W., Yim, J., Bruno, M., Snyder, T., Reust, T., Mainau, L., Garvey, W.T., and Morré, D.J. Isolation by preparative free-flow electrophoresis and aqueous two-phase partition from rat adipocytes of an insulin-responsive small vesicle fraction with glucose transport activity. *J. Chromatog.*, vol. 680, 201-212 (1996).
- Moya-Camarena, S., Morré, D.J., and Morré, D.M. Isolation and characterization of Golgi apparatus from transformed cell lines in culture. *Mol. Biol. Cell*, vol. 6, no. 328a, (1995).
- Muschol, M., and Rosenberger, F. "Absence of prenucleation aggregation in lysozyme solutions - Static and dynamic light scattering results." *Sixth International Conference on Crystallization of Biological Macromolecules*, Hiroshima, Japan, November 1995.

- Muschol, M., and Rosenberger, F. Interactions in undersaturated and supersaturated lysozyme solutions: Static and dynamic light scattering results. *J. Chem. Phys.*, vol. 103, 10424-10432 (1995).
- Muschol, M., and Rosenberger, F. "Light scattering investigation of phase transitions in lysozyme solutions." International Laser Light Scattering Symposium, Hong Kong, July 1996.
- Muschol, M., and Rosenberger, F. "Is the shape of phase diagrams for globular proteins universal?" Photon Correlation and Scattering Topical Meeting, Capri, Italy, August 1996.
- Muschol, M., and Rosenberger, F. "Liquid phase separation in lysozyme." Workshop on Response Surface Methods in Protein Crystallization, Univ. of North Carolina, Chapel Hill, June 1996.
- Nakashima, M. and Martin, A. "Clonal T-cell response to hTSHR-peptide revealed by radio-labelled PCR." *Thyroid* 5 (Supplement 1): 41, 11th International Thyroid Congress, Toronto, Canada, September 10-15, 1995.
- Nakashima, M., Martin, A., and Davies T.F. Intrathyroidal T-cell accumulation in Graves' disease: delineation of mechanisms based on in situ T-cell receptor analysis. *Journal of Clinical Endocrinology and Metabolism*, 81:3346-3335 (1996).
- O'Connor, K.C. Cultivating insect cells to produce recombinant proteins. NASA Tech Brief, 20, 79 (1996).
- O'Connor, K.C., Enmon, R.M., Dotson, R.S., Primavera, A.C., and Clejan, S. Characterization of autocrine growth factors, their receptors and extracellular matrix present in three-dimensional cultures of DU 145 human prostate carcinoma cells grown in simulated microgravity. *Tissue Eng.*, Submitted, (1996).
- O'Connor, K.C., Enmon, R.M., Primavera, A.C., Dotson, R.S., and Clejan, S. "Characterization of extracellular matrix in three-dimensional cultures of DU 145 human prostate carcinoma cells." *Animal Cell Technology: From Vaccines to Genetic Medicine*. Kluwer Academic Publishers, Dordrecht, In Press, 1996.
- O'Connor, K., Clejan, S., Cowger, N., Enmon, R., Dotson, R., and Primavera, A. "Effects of simulated microgravity on DU 145 human prostate carcinoma cells." Spring Meeting of the American Chemical Society, New Orleans, LA, 1996.
- O'Connor, K., Clejan, S., Cowger, N., Enmon, R., Dotson, R., and Primavera, A. "Effects of simulated microgravity on DU 145 human prostate carcinoma cells." Cancer Association of Greater New Orleans, New Orleans, LA, 1996.
- O'Connor K, Clejan S, Enmon R, Rosenzweig N, Dotson R, and Primavera A. "Characterization of autocrine regulatory processes in DU 145 human prostate carcinoma cells." Annual Meeting of the American Institute of Chemical Engineers, Chicago, IL, 1996.
- O'Connor, K., Enmon, R., Primavera, A., Dotson, R., and Clejan, S. "Characterization of growth factors and extracellular matrix in three-dimensional cultures of DU 145 human prostate carcinoma cells." Meeting of the European Society for Animal Cell Technology, Vilamoura, Portugal, 1996.
- O'Connor, K., Rosenzweig, N., and Clejan, S. Simulated microgravity inhibition of in vitro aggressiveness of prostate cancer is accompanied by changes in signal transduction and lipid second messengers. *FASEB J.*, 10, A1396 (1996).
- Obitz, T.W. "Mechanical properties of articular cartilage and tissue engineered constructs: a transversely isotropic analysis." S.M Thesis, Boston University, Boston, MA, Vunjak-Novakovic G on Thesis Committee, Stamenovic D, Advisor, September, 1996.
- Obitz, T.W., Eisenberg, S.R., and Stamenovic, D. "Creep Behavior of Calf Articular Cartilage: a Transversely Isotropic Analysis." Annual Meeting of the BMES, University Park, PA. October, 1996.
- Osterberg, E., Bergstrom, K., Holmberg, K., Schuman, T.P., Riggs, J.A., Burns, N.L., Van Alstine, J.M., and Harris, J.M. Protein rejecting ability of surface bound dextran in end-on and side-on configurations. *J. Biomed. Materials Res.*, vol. 29, 741-747 (1995).
- Pellis, N.R. "Establishment of 3-dimensional primary hepatocyte cultures in microgravity environment." *Amer. Assoc. for the Study of Liver Diseases*, 11/3-11/7/95, Chicago, IL. *Hepatology*, Vol. 22, No. 4, Pt. 2, P. 231A (Abst. #498), 1995.

- Pellis, N.R. "Biotechnology and Space Research." University of Houston, Clear Lake, Houston, Texas, November 3, 1995.
- Pellis, N.R. "Research Update: Microgravity and Immunosuppression." Gillison-Longbaugh Foundation, Houston, Texas, November 7, 1995.
- Pellis, N.R. "Biomedical research in space." Tulare County Medical Society, Visalia, California, February 16, 1996.
- Pellis, N.R. "Microgravity and Immunosuppression: A Ground-based Model in the Slow Turning Lateral Vessel Bioreactor." Investigators Working Group (IWG), Houston, Texas, February 24, 1996.
- Pellis, N.R. "Cell Biology in Space." San Jacinto College, Houston, Texas, March 4, 1996.
- Pellis, N.R., Ellis, L., and Balch, C.M. "Tumor Biology". In: "Surgery: Scientific Principles and Practice." Philadelphia: JB Lippincott, 1996.
- Pellis, N.R., Goodwin, T.J., Risin, D., McIntyre, B.W., Pizzini, R.P., Cooper, D., Prewett, T.L., and Spaulding, G.F. Randomization of gravitational vectors inhibits human lymphocyte locomotion through type I collagen. *In Vitro*. (In Press).
- Peng, C.A. and Palsson, B.O. Cell Growth and Differentiation on Feeder Layers is Predicted to be Influenced by Bioreactor Geometry. *Biotechnology and Bioengineering*, Vol. 50, 479-492 (1996).
- Peng, C.A. and Palsson, B.O. Importance of Nonhomogeneous Concentration Distributions Near Walls in Bioreactors for Primary Cell Cultures. *Ind. Eng. Chem. Res.*, Vol. 34, 3239-3245 (1996).
- Peng, C.A., Koller, M.R., and Palsson, B.O. Unilineage Model for Hematopoiesis Predicts Self-Renewal of Stem and Progenitor Cells from Observed Ex Vivo Growth Patterns. *Biotechnology and Bioengineering*, 52:24-33 (1996).
- Pinelli, D., Cavanagh, D., and Becker, J. Hormonal modulation of Ishikawa cells during three-dimensional growth in vitro. *Soc. Gynecol. Oncol.*, (Submitted).
- Rhiel, M., Murhammer, D., Zhou, X., and Arnold, M. "Cell culture process monitoring by NIR spectroscopy." *Pittcon'96*, Chicago, IL, March 5, 1996.
- Rhiel, M., Riley, M., Zhou, M., Arnold, M., and Murhammer, D. "Sensitivity and selectivity of near-infrared spectroscopy methods for process monitoring." *AIChE National Meeting*, Chicago, IL, November, 1996.
- Richardson, J.S., Richardson, D.C., LaBean, T.H., Gernert, K.M., and Word, M.J. "The Problem of Unique vs. Approximate Structures in Protein Design (invited lecture)." *International Conference on Protein Folding and Design*, National Institutes of Health, Bethesda, Maryland, April 23-26, 1996.
- Richardson, J.S., Richardson, D.C., LaBean, T.H., Gernert, K.M., and Word, M.J. "The Problem of Unique vs. Approximate Structures in Protein Design (poster presentation)." *The Johns Hopkins Protein Folding Meeting*, Coolfont, Berkeley Springs, West Virginia, March 16-19, 1996.
- Riley, M., Arnold, M., and Murhammer, D. "Non-invasive measurement of glucose concentrations by near infrared spectroscopy." *Biomedical Engineering Society Fall Meeting*, State College, Pennsylvania, 1996.
- Riley, M., Rhiel, M., Arnold, M., and Murhammer, D. "Monitoring metabolite concentrations in insect and mammalian cell bioreactors by NIR spectroscopy." *AIChE National Meeting*, Chicago, IL, November, 1996.
- Riley, M., Rhiel, M., Zhou, X., Arnold, M., and Murhammer, D. Simultaneous measurement of glucose and glutamine in insect cell culture media by near-infrared spectroscopy. *Biotechnology and Bioengineering*, (In Press).
- Risin, D., Kleinerman, E.S., Umezu, Y., Pizzini, P.R., Valch, C.M., and Pellis, N.R. Impairment of lymphocyte locomotion in the tumor microenvironment and the effect of systemic immunotherapy with L-MTP-PE. *Cancer Immunol. Immunother.*, 40:57-64, (1995).

- Risin, D., Prewett, T.L. and Pellis, N.R. Suppression of lymphocyte function in microgravity and potential impact on immunosurveillance. Abstracts of the Fifth International Conference on Anticancer Research, October 17-22, 1995, Corfu, Greece. Anticancer Res., Vol 15, Number 5A, 1652 (Abst #72) (Sept-Oct 1995).
- Rosenbaum, D.F. and Zukoski, C.F. Protein interactions and crystallization. J. Crystal Growth, vol. 169, 752 (1996).
- Rosenbaum, D., Zamora, P.C., and Zukoski, C.F. Phase behavior of small attractive particles. Phys. Rev. Letters, vol. 76, no. 150, (1995).
- Rosenberger, F. "Nucleation and crystallization of globular proteins - what do we know and what is missing?" Sixth International Conference on Crystallization of Biological Macromolecules, Hiroshima, Japan, November 1995.
- Rosenberger, F. Protein crystallization. J. Crystal Growth, vol. 166, 40-54 (1996).
- Rosenberger, F. "Protein crystallization." Sixth Eastern Regional Conference on Crystal Growth, Atlantic City, New Jersey, October 1995.
- Rosenberger, F. "Interaction between bulk transport and interface kinetics in crystal growth from solutions." Second European Symposium on Fluids in Space, Naples, Italy, April 1996.
- Rosenberger, F. "Physical chemistry of globular protein crystallization." Gordon Research Conference on Diffraction Methods in Molecular Biology, Proctor Academy, Andover, New Hampshire, June 1996.
- Saltzman, W.M. Growth factor delivery in tissue engineering. MRS Bulletin, (In Press).
- Saltzman, W.M. "Cell Interactions with Polymers," in "Textbook of Tissue Engineering." Edited by: Lanza RP, Chick WL and Langer R (Ed.) Springer, NY, pp 227-248, 1996.
- Schall, C., Arnold, E., and Wiencek, J.M. Enthalpy of Crystallization of Hen Egg White Lysozyme. J. Cryst. Growth, vol. 165, 293 (1996).
- Schall, C., Bonita, J., Li, E., Arnold, E., and Wiencek, J.M. Application of temperature control strategies to the growth of hen egg-white lysozyme crystals. J. Cryst. Growth, vol. 165, 299 (1996).
- Smith, C.D. "Scenarios for handling Crystals Onboard Space Station." Macromolecular Crystallization Meeting, Panama City, Florida, April 29, 1996.
- Sportiello, M.G., Todd, P., Lee, C.-Y., Kundrot, C.E., Schultz, S., Stodieck, L.S., and Cassanto, J.M. "High frequency access to low gravity experimentation in organic crystal growth from solutions." Proc. Space 96, 5th International Conference on Engineering, Construction and Operations in Space, Albuquerque, New Mexico, June 2-6, 1996.
- Stayton, P. "Proteins at Interfaces." University of Wisconsin, November 1995.
- Stayton, P. "Engineering molecular recognition events at biomaterial interfaces." Naval Research Laboratory Workshop on Non-Biomedical Applications of Biomaterials, August 1996.
- Stayton, P. "Molecular recognition in the streptavidin-biotin system." Georgetown University, April 1996.
- Stayton, P. "Proteins at Interfaces." Biorecognition at Interfaces Symposium at the 70th Colloid and Surface Science Symposium, American Chemical Society, June 1996.
- Stayton, P. "Proteins at Interfaces." Duke University, April 1996.
- Sygyusch, J., Coulomb, R., Cassanto, J.M., Sportiello, M.G., and Todd, P. Protein crystallization in low gravity using a novel liquid-liquid diffusion method. J. Crystal Growth, vol. 162, 167-172 (1996).
- Thomas, B.R., and Rosenberger, F. "Heterogeneity determination and purification of commercial hen egg white lysozyme." Protein Crystal Growth Conference, Panama City, Florida, April 1996.

- Thomas, B.R., Vekilov, P.G., and Rosenberger, F. Heterogeneity determination and purification of commercial hen egg white lysozyme. *Acta Cryst. D*, vol. 52, 776-784 (1996).
- Tiede, D.M., and Thiyagarajan, P. "Characterization of photosynthetic supramolecular assemblies using small angle neutron scattering (in "Biophysical Techniques in Photosynthesis")." Edited by: J. Ames and A.J. Hoff Kluwer Academic Publishers, Dordrecht, pp 375-390, 1996.
- Tiede, D.M., Marone, P., Wagner, A.M., and Thiyagarajan, P. "Characterization of photosynthetic supramolecular assemblies using small angle neutron scattering (in "Photosynthesis: from light to biosphere")." Edited by: P. Mathis Kluwer Academic Publishers, Dordrecht, pp 431-436, 1995.
- Todd, P. "Analysis of crystallization by osmotic dewatering and its application to oligonucleotides." Protein Crystal Growth Conference, Panama City Beach, Florida, April 28-30, 1996.
- Trinh, E.H. "Development of a Rotating Levitated Drop Apparatus for Crystal Growth from Solution." 1996 Protein Crystal Growth Conference, Panama Beach City, Florida, April 28-30, 1996.
- Van Alstine, J.M. "Phase partitioning on earth and in space." Department of Biochemistry, University of Lund, Sweden, Spring 1995.
- Van Alstine, J.M. "Polymer coated surfaces and proteins (invited presentation)." Immunex Corporation, Seattle, Washington, October 26, 1995.
- Van Alstine, J.M. "Polymer coated surfaces for improved biosensors (invited presentation)." Pharmacia Biosensor, Uppsala, Sweden, November 9, 1995.
- Van Alstine, J.M. "Polymer coatings of significance in low gravity bioprocessing (invited presentation)." NASA/MSFC Space Science Lab, Huntsville, Alabama, January 10, 1996.
- Van Alstine, J.M. "Polymer coatings and improved biochemical analyses (invited presentation)." Astra Hässle, Göteborg, Sweden, February 22, 1996.
- Van Alstine, J.M.. "Polymer coated surfaces of pharmaceutical significance (invited presentation)." Nycomed AS, Oslo, Norway, February 29, 1996.
- Van Alstine, J.M., and Malmsten, M. "Poly(ethylene glycol) amphiphiles." Industrial Symposium on Surface Chemistry: Wetting and Flocculation, Oslo, Norway, November 8-9, 1995.
- Van Alstine, J.M., Malmsten, M., and Brooks, D.E. Poly(ethylene glycol) amphiphile adsorption and liposome partition. *J. Chromatog.*, vol. 680, 145-155 (1996).
- Van Alstine, J.M., Veide, A., and Tjerneld, F. Phase partition and biotechnology. *Trends Biotech.*, vol. 16, 1-3 (1996).
- Vekilov, P.G., Alexander, J.I.D., and Rosenberger, F. "Unsteady dynamics of layer growth in the mixed kinetics-bulk transport regime." Tenth American Conference on Crystal Growth, Vail, Colorado, August 1996.
- Vekilov, P.G., and Rosenberger, F. "Impurities, growth layer sources and kinetics fluctuations in the growth of lysozyme crystals."
- Vekilov, P.G., and Rosenberger, F. Dependence of lysozyme growth kinetics on step sources and impurities. *J. Crystal Growth*, vol. 158, 540-551 (1996).
- Vekilov, P.G., and Rosenberger, F. "New factors for protein crystal perfection on Earth and under reduced gravity." Protein Crystal Growth Conference, Panama City, Florida, April 1996.
- Vekilov, P.G., Monaco, L.A., and Rosenberger, F. Facet morphology response to nonuniformities in nutrient and impurity supply. I. Experiments and interpretation. *J. Crystal Growth*, vol. 156, 267-278 (1995).

- Vekilov, P.G., Monaco, L.A., Thomas, B.R., Stojanoff, V., and Rosenberger, F. "Impurity- and salt-rich coring in lysozyme crystals." Sixth International Conference on Crystallization of Biological Macromolecules, Hiroshima, Japan, November 1995.
- Vekilov, P., Monaco, L.A., Thomas, B.R., Stojanoff, V., and Rosenberger, F. Repartitioning of NaCl and protein impurities in lysozyme crystallization. *Acta Cryst. D*, vol. 52, 785-798 (1996).
- Vogel, V. "Two-dimensional protein crystallization at interfaces." Max-Planck Institute for Polymer Research, Mainz, Germany, July 1996.
- Vogel, V. "Two-dimensional protein crystallization at interfaces." Technische Universität, München, Germany, July 1996.
- Vogel, V. "Surface recognition to orient, crystallize and direct the motility of proteins at interfaces." Gordon Conference on Biomolecular Recognition and Immobilization, August 1996.
- Vogel, V. "2-D protein crystals." Summer School of the Laboratory for Exotic Nanomaterials, Riken Frontier Research Institute, Wako, Japan, August 1996.
- Vogel, V. "Langmuir monolayers as model for the study of early nucleation events." Workshop on Molecular Engineering of Inorganic Materials at Organic Interfaces, Friday Harbor, Washington, September 1996.
- Vogel, V., Frey, W., Schief, Jr., W.R., and Stayton, P.S. "Critical surface density and protein/protein contacts in 2-D protein crystallization." Protein Crystallization Conference, Panama City Beach, Florida, April 1996.
- Vogel, V., Frey, W., Schief, Jr., W.R., Chilkoti, A., and Stayton, P.S. "Dynamics of Protein Aggregation and Crystallization at Interfaces." MRS Meeting, Boston, Massachusetts, November 27 - December 1, 1995.
- Vunjak-Novakovic, G. and Freed, L. Cell-polymer system for tissue engineering. *Chemical Industry*, 49, (12)511-519 (1996).
- Vunjak-Novakovic, G. and Freed, L.E. Cell-polymer system for tissue engineering. *Chemical Industry*, 49 (12), 511-519 (1996).
- Vunjak-Novakovic, G., Freed, L.E., and Langer, R. Chondrocytes cultured on biodegradable polymers. *Synovial I. Rheumatologie*, 4-5 (April 1996).
- Vunjak-Novakovic, G., Freed, L.E., and Langer, R. "Bioreactor Cultivation of Chondrocytes on Biodegradable Polymer Scaffolds." 5th World Congress of Chemical Engineering, San Diego, CA, July 1996.
- Vunjak-Novakovic, G., Freed, L.E., and Langer, R. "Chondrocytes Cultured on Biodegradable Polymers." *Interventional Rheumatology: From Basic to Clinical Research*, Paris, France, March 1996.
- Vunjak-Novakovic, G., Freed, L.E., and Langer, R. "Effects of Hydrodynamic Forces on Natural and Tissue Engineered Cartilage." Annual Meeting of the BMES, Boston, MA, October 1995. 23:S-59.
- Vunjak-Novakovic, G., Freed, L.E., and Langer, R. Chondrocytes cultured on biodegradable polymers. *Synovial J. Rheumatologie*, 4-5 (April 1996).
- Vunjak-Novakovic, G., Freed, L.E., and Langer, R. "Bioreactor Cultivation of Chondrocytes on Biodegradable Polymer Scaffolds." 5th World Congress of Chemical Engineering, San Diego, CA. July, 1996.
- Vunjak-Novakovic, G., Freed, L.E., and Langer, R. "Chondrocytes Cultured on Biodegradable Polymers." *Interventional Rheumatology: From Basic to Clinical Research*, Paris, France. March, 1996.
- Vunjak-Novakovic, G., Freed, L.E., and Langer, R. "Effects of Hydrodynamic Forces on Natural and Tissue Engineered Cartilage." Annual Meeting of the BMES, Boston, MA. October 1995. 23:S-59.
- Vunjak-Novakovic, G., Freed, L.E., Biron, R.J., and Langer, R. Effects of mixing on tissue engineered cartilage. *American Institute of Chemical Engineers Journal (AIChEJ)*, 42, 850-860 (1996).

- Vunjak-Novakovic, G., Freed, L.E., Biron, R.J., and Langer, R. Effects of mixing on tissue engineered cartilage. American Institute of Chemical Engineers Journal (AIChEJ), 42:850-860 (1996).
- Wiedemeier, H., and Hutchins, M.A. The Temperature-Composition Phase Equilibria in the HgTe-Hgl₂ Pseudobinary System. Z. anorg. allg. Chem., vol. 622, 1150-1160 (1996).
- Wiencek, J.M. "Protein Crystallization: Microcalorimetric Investigations & Thermally Controlled Growth." NASA Protein Crystal Growth Conference, Panama City Beach, Florida, April 1996.
- Wiencek, J.M. "Effect of DMSO on Peroxidase-Catalyzed Polymerization of Cresol." U.S. Army Edgewood Research, Development, and Engineering Center Scientific Conference on Chemical Defense Research, November 15, 1995.
- Wilson, W. "The Second Virial Coefficient as a Predictor in Protein Crystal Growth." 211th American Chemical Society National Meeting, New Orleans, Louisiana, March 1996.
- Wilson, W. "The Second Virial Coefficient as a Predictor in Protein Crystallization." Protein Crystal Growth Conference, Panama City, Florida, April 1996.
- Yin, Y., and Carter, Jr., C.W. Incomplete Factorial and Response Surface Methods in Experimental Design: Yield Optimization of tRNA^{Trp} from *in vitro* T7 RNA Polymerase Transcription. Nucl. Acids. Res., vol. 24, 1279-1287 (1996).
- Zhau, H.E., Goodwin, T.J., Chang, S.M., Baker, T.L., and Chung, L.W.K. Establishment of a 3-dimensional human prostate organoid co-culture under microgravity-simulated condition: Evaluation of androgen-induced growth and PSA expression. In Vitro, In Press, (July 26, 1996).
- Zhou, X., Arnold, M., Murhammer, D., and Rhiel, M. "Feasibility of on-line bioreactor monitoring by near infrared spectroscopy." Federation of Analytical Chemistry and Spectroscopy Societies, Cincinnati, Ohio, October 15, 1995.
- Zukoski, C.F., Rosenbaum, D.F., and Zamora, P.C. Aggregation in precipitation reactions: Stability of primary particles. Trans. of the Inst. of Chem. Engin., Part A, vol. 74, 723 (1996).

Ground: Combustion Science

- Abbud-Madrid, A., Branch, M.C., and Daily, J.W., On the burning behavior of radiatively ignited titanium at low gravity. AIAA Paper 96-0262, (Jan 15-18, 1996).
- Abbud-Madrid, A., Branch, M.C., and Daily, J.W., "Ignition and combustion of bulk titanium and magnesium at normal and reduced gravity." 26th International Symposium on Combustion, The Combustion Inst., Naples, Italy, Paper 443, July 29-Aug. 2, 1996.
- Abbud-Madrid, A., Branch, M.C., and Daily, J.W., Ignition and combustion of bulk metals at normal, elevated, and reduced gravity. Univ. of Colorado Report CCR No. 95-05 - Annual Technical Report, (CASI N96-17775), NASA CR-200007, (December 10, 1995).
- Aharon, I. and Shaw, B.D. "Combustion of heptane/hexadecane mixture droplets in reduced gravity at sub-atmospheric, atmospheric and elevated pressures." Western States Section of the Combustion Institute, Fall meeting, Stanford, CA., paper #WSS 95F-226, November, 1995.
- Aharon, I., Shaw, B.D., "Marangoni instability of bi-component droplet gasification in reduced gravity." Western States Section of the Combustion Institute, Fall Meeting, Stanford, CA, paper #WSS 95F-227, November, 1995.
- Aharon, I., Shaw, B.D., Gage, J.J., Jenkins, A.J., and Kahoe, T.J., "Combustion of alcohol mixture droplets in reduced gravity." Western States Section of the Combustion Institute, Fall meeting, Stanford, CA, paper #WSS 95F-228, November, 1995.
- Aharon, I., Shaw, B.D., Gage, J.W., Jenkins, A.J., and Kahoe, T.K., Combustion of alcohol mixture droplets in reduced gravity. Combustion Science and Technology, (1996).

Aharon, I., Shaw, B.D., Gage, J.W., Jenkins, A.J., and Kahoe, T.K., "Combustion of alcohol mixture droplets in reduced gravity." presented at the 1995 Fall Meeting of the Western States Section of the Combustion Institute, paper WSS 95F-228, Stanford, CA., 1995.

Al-Ammar, K.N., Agrawal, A.K., and Gollahalli, S.R., "Quantitative measurements in hydrogen flames by rainbow Schlieren imaging." presented at the meeting of the Central States Section of the Combustion Institute, May 5-7, 1996.

Aldushin, A.P., Matkowsky, B.J., and Schult, D.A., Downward buoyant filtration combustion. Combustion and Flame, (accepted 1996).

Aldushin, A.P., Matkowsky, B.J., and Volpert, V.A., Enhancement of gasless combustion synthesis by counterflow gas filtration. Combustion Science and Technology, vol. 103, pp. 1-20 (October 1995).

Atreya, A., Zhang, C., Kim, H.K., Shamim, T., and Suh, J., "The effect of change in the Flame structure on formation and destruction of soot and NO_x in radiating diffusion flames." presented to the 26th International Combustion Symposium, Naples Italy, 1996.

Axelbaum, R.L., Huertas, J.I., Lottes, C.R., Hariprasad, S., Sastry, S.M.L., "Nanophase W and W-Ti composite via gas-phase combustion synthesis." 1996 ASME Mechanics and Materials Conference, Johns Hopkins University, Baltimore, June 12-14, 1996.

Axelbaum, R.L., Lottes, C.R., Huertas, J.I. and Hariprasad, S., "Gas-phase combustion synthesis of aluminum nitride powders." Proceedings of the 26th Symposium (International) on Combustion, Naples, Italy, July 1996.

Axelbaum, R.L., Lottes, C.R., Huertas, J.I. and Hariprasad, S., "Gas-phase combustion synthesis of aluminum nitride powders." presented at the 26th Symposium (International) on Combustion, Naples, Italy, July 1996.

Axelbaum, R.L., Lottes, C.R., Huertas, J.I., Rosen, L.J. and Hariprasad, S., "Synthesis of aluminum nitride nano-particulates via gas-phase combustion." Third International Conference on Nanostructured Materials, Kona, Hawaii, July 8-12, 1996.

Axelbaum, R.L., Lottes, C.R., Huertas, L.J. and Hariprasad, S., "Gas-phase combustion synthesis of nano-particulates of W and W-Ti composite." Third International Conference on Nanostructured Materials, Kona, Hawaii, July 8-12, 1996.

Bang, H.-N., An experimental investigation of jet diffusion flames: flame response and stabilization in cross-flow, M.S. Thesis. The University of Iowa, Iowa City, Iowa, (July, 1996).

Bang, H.-N. and Chen, L.-D., "An experimental investigation of laminar jet diffusion flame stabilization in cross-flow." Proceedings of the 1996 Spring Technical Meeting of the Central States Section of The Combustion Institute, St. Louis, MO, pp. 175-280, May 5-7, 1996.

Boratav, O., Elghobashi, S., and Zhong, R., On the alignment of alpha-strain and vorticity in nonpremixed flames. Physics of Fluids, vol. 8 (8), 2251-2253 (August 1996).

Boratav, O., Elghobashi, S., and Zhong, R., "Buoyancy effects on the structure of turbulence in nonpremixed flames." Proceedings of the SIAM - 6th International Conference on Numerical Combustion, New Orleans, March 4-6, 1996.

Branch, M.C., Daily, J.W., and Abbud-Madrid, A., Ignition and combustion of bulk metals in a microgravity environment. NASA Tech Brief, CCR No. 96-09, (September 16, 1996).

Buckmaster, J., "Modeling microgravity combustion phenomena." Invited Plenary Lecture, The Eastern States Meeting of the Combustion Institute, October 16-18, 1995.

Buckmaster, J., "Smoldering combustion." AIAA 96-0258, AIAA 34th Aerospace Sciences Meeting & Exhibit, Reno, NV, 1996.

Buckmaster, J., "Edge-flame-holding." Proceedings of the 26th Symposium (International) on Combustion, Naples, Italy, July 1996.

Buckmaster, J., A theory of shallow smolder waves. IMA J. of Applied Mathematics, vol. 56, pp. 87-102 (1996).

- Buckmaster, J., Edge-flames and their stability. Comb. Sci. & Technol., vol. 115, pp. 43 (1996).
- Buckmaster, J., "Modeling microgravity combustion phenomena." Invited Plenary Lecture, The Eastern States Meeting of the Combustion Institute, October 16-18, 1995.
- Buckmaster, J., "Smouldering combustion." AIAA 96-0258, AIAA 34th Aerospace Sciences Meeting & Exhibit, Reno, NV, 1996.
- Buckmaster, J., "Applications of a one-dimensional model of edge-flames." Combustion Problems session, the 19th International Congress of Theoretical and Applied Mechanics, Kyoto, Japan, August 25-31, 1996.
- Buckmaster, J., and Lozinski, D., "Extinction and other topics in smouldering combustion." Proceedings of the Third Asian-Pacific Int. Symp. on Combustion and Energy Utilization, Vol. II, Combustion Fundamentals, pp. 426-431, Hong Kong, December 1995.
- Buckmaster, J., and Lozinski, D., An elementary discussion of forward smoldering. Combustion and Flame, vol. 104, pp. 300-310 (1996).
- Buckmaster, J. and Weber, R., "Edge-flame-holding." presented at the 26th Symposium (International) on Combustion, Naples, Italy, July 1996.
- Buckmaster, J. D., "Radiation losses in hydrogen-air flame-balls, combustion fundamentals and applications." Proceedings of the Central States Section of The Combustion Institute, pp. 316-321, 1996, St. Louis, Missouri, May 5-7, 1996.
- Buckmaster, J. D., "Radiation losses in hydrogen-air flame-balls." Combustion Fundamentals and Applications, Proc. of the Central States Section of The Combustion Institute, pp. 316-321, 1996, St. Louis, Missouri, May 5-7, 1996.
- Cheatham, S. and Matalon, M., "Near-Limit Oscillations of Spherical Diffusion Flames ." AIAA Paper 96-0260, 34th Aerospace Sciences Meeting and Exhibit, 1996.
- Cheatham, S. and Matalon, M., Near-limit oscillations of spherical diffusion flames. AIAA Journal, (1996).
- Cheatham, S. and Matalon, M., "Heat Loss and Lewis number effects on the onset of oscillations in diffusion flames ." Twenty-Sixth Symposium (International) on Combustion, 1996.
- Chen, G. and Gomez, A., "Group combustion of a dilute spray in a co-flow laminar diffusion flame." Proceedings of the Third Asian-Pacific International Symposium on Combustion and Energy Utilization, Hong Kong, vol. 2, p. 384, December 11-15, 1995.
- Chen, G. and Gomez, A., Co-flow laminar diffusion flames of monodisperse sprays: structure, evaporation and microgravity effects. Combust. Sci. and Tech., 115, p. 199 (1996).
- Chen, G. and Gomez, A. "Group combustion in co-flow laminar diffusion flame." presented at the 1995 Technical meeting Eastern States Section of the Combustion Institute, Worcester, MA, October 1995.
- Chen, G. and Gomez, A., "Co-flow laminar diffusion flames of monodisperse sprays: structure, group combustion and microgravity effects." Paper 95-F70 presented at the 1995 Fall Meeting of the Western States Section/The Combustion Institute, Stanford CA, October 1995.
- Chen, G. and Gomez, A., "Recent Advances in Spray Combustion, Chapter Title: The structure of a co-flow laminar diffusion flame." Edited by: K.Kuo, Ed AIAA Book Series, October 1995.
- D'Angelo, Y., Silverman, I., Gao, L.P., Gomez, A. and Smooke, M.D., "Computational and experimental study of counterflow spray diffusion flames." presented at the 1995 Technical Meeting of the Eastern States Section / The Combustion Institute, Worcester, MA, October 1995.
- DiCicco, M., and Buckmaster, J., Role of slip in the generation of acoustic instabilities in gas turbines. J. of Propulsion and Power, vol. 12, no. 1, pp. 34-40 (1996).

Dreizen, E.L., Experimental study of stages in aluminum particle combustion in air. Comb. and Flame, vol. 105, pp. 541-556 (June 1996).

Dreizen, E.L. and Calcote, H.F., "A new mechanism of boron ignition: Through the formation of a saturated B-O solution." Paper presented at the Fall Tech. Meeting of the Eastern States Sec., The Combustion Inst., Worcester MA, October, 1995.

Egolfopoulos, F.N., Zhang, H. and Zhang, Z., Wall effects on the propagation and extinction of strained, laminar, premixed flames. Combustion and Flame, (February, 1996).

Egolfopoulos, F.N., Zhang, H., Vagelopoulos, C.M., and Zhang, Z. "Dynamic and stability effects on counterflowing laminar premixed flames: Implications on the determination of laminar flame speeds." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28-August 2, 1996.

Egolfopoulos, F.N., Zhang, H., Zhang, Z., and Kastanas, G., "Wall effects on the propagation and extinction of strained, laminar, premixed flames." Fall Meeting, Western States Section of the Combustion Institute, Stanford University, Palo Alto, California, Paper No. 95F-215, October 30-31, 1995.

Elghobashi, S., Boratav, O. and Zhong, R., "Effects of buoyancy on turbulent nonpremixed flames." Invited lecture at the International Conference on Turbulent Heat Transfer, San Diego, March 10-15, 1996.

Elghobashi, S., Boratav, O.N., and Zhong, R., Effects of buoyancy on turbulent nonpremixed flames. Bulletin of APS, vol. 40 (12), 1991 (October 1995).

Faeth, G.M. and Koyle, U.O., "Structure and optical properties of flame-generated soot." Proceedings of the 8th International Symposium on Transport Phenomena in Combustion. November, 1995.

Fisher, I., Buckmaster, J., Lozinski, D. and Matalon, M., Vapor diffusion flames, their stability, and annular pool fires. Mathematical Modeling in Combustion Science, Springer Verlag, pp. 249-257 (1995).

Gao, L.P., D'Angelo, Y., Silverman, I., Gomez, A. and Smooke, M.D., "Quantitative comparison of detailed numerical computations and experiments in counterflow spray diffusion flames." Paper presented at the Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28 to August 2, 1996.

Haggard, B., Dryer, F.L., Nayagam, V., Shaw, B.D., and Williams, F.A., "Droplet combustion experiments in spacelab." Twenty-Sixth Symposium (International) on Combustion, Naples, Italy, 1996.

Haggard, J.B. Dryer, F.L., Nayagam, V., Shaw, B.D., and Williams, F.A., "Droplet combustion experiments in spacelab." Twenty-Sixth Symposium (International) on Combustion, Naples, Italy, 1996.

Haggard, J.B., Dryer, F.L., Nayagam, V., Shaw, B.D., and Williams, F.A., "Droplet combustion experiments in spacelab." Twenty-Sixth Symposium (International) on Combustion / The Combustion Institute, 1996.

Haggard, J.B., Dryer, F.L., Nayagam, V., Shaw, B.D., and Williams, F.A., Droplet combustion experiments in spacelab. The Combustion Institute, (1996).

Haggard, J.B., Dryer, F.L., Nayagam, V., Shaw, B.D., and Williams, F.A., "Droplet combustion experiments in spacelab." Twenty-Sixth Symposium (International) on Combustion, Naples, Italy, 1996.

Hertzberg, J., Carlton, J., Bradley, E., Luff, J., and Linne, M., "A split, bifurcated diffusion flame." Presentation HF5 at the 48th Annual Division of Fluid Dynamics, American Physical Society Meeting, November 19-21, Irvine, CA. Abstract published in Bull. APS Volume 40, no. 12, pp. 2015, October 1995.

Hertzberg, J., Carlton, J., Schweiterman, M., Bradley, L., and Linne M., "Splitting of an axially excited jet diffusion flame." Work-In-Progress Poster 2-017 at the 26th International Symposium on Combustion, Naples, Italy, July 29-August 2, 1996.

Hertzberg, J.R., Conditions for a split diffusion flame. Combustion and Flame, (September 1995).

- Honda, L. and Ronney, P.D., "Mechanisms of concurrent-flow flame spread over thin solid fuels." presented at the Fall Technical Meeting of the Western States Section of the Combustion Institute, Stanford, CA, October 30-31, 1995.
- Jaeleson, G.S. and Avedisian, C.T. Modeling of spherically symmetric droplet flames including complex chemistry: Effect of water addition on n-heptane droplet combustion. *Combustion Science and Technology*, vol. 115, pp. 125-149 (1996).
- Karpetis, A. N. and Gomez, A., Temperature measurements in spray flames using spontaneous raman scattering. *Optics Letters*, 21, p. 704 (1996).
- Karpetis, A. N. and Gomez, A., "Gas temperature measurements by Stokes/Anti-Stokes raman thermometry in spray flames." presented at the 1995 Technical Meeting of the Eastern States Section / The Combustion Institute, Worcester, MA, October 1995.
- Ku, J.C., Toug, L., and Greenberg, P.S. "Detailed modeling analysis for soot formation and radiation in microgravity gas jet diffusion flames." Third International Microgravity Combustion Workshop, Cleveland, OH, April 11-13, 1995.
- Ku, J.C., Toug, L., and Greenberg, P.S. Measurements and modeling of soot formation and radiation in microgravity jet diffusion flames. HTD-vol.335 Proceedings of the ASME Heat Transfer Division, vol. 4, (1996).
- Lee, Y.G. and Chen, L.-D., "Effects of Damkohler number on the lifted methane laminar diffusion flames at reduced pressure." presented at the KSEA 6th Midwest Regional Conference, Iowa City, Iowa, June 21-22, 1996.
- Lin, K.-C., Sunderland, P.B., and Faeth, G.M., Soot nucleation and growth in laminar acetylene/air diffusion flames. *Combustion and Flame*, (1996).
- Lozinski, D., and Buckmaster, J., Quenching of reverse smolder. *Combustion and Flame*, vol 102, pp.87-100 (October 1995).
- Luff, J., "Uncertainties associated with the post-processing of 2-D particle imaging velocimetry (PIV) velocity data in unsteady flow fields." Colorado School of Mines thesis no. T-4831, November 1995.
- Luff, J.D., Rompage, A.M., Linne, M.A., and Hertzberg, J.R., Uncertainties associated with the post-processing of 2-D particle imaging velocimetry (PIV) velocity data of unsteady flow fields. *Experiments in Fluids*, (August 1996).
- Luff, J.D., Rompage, A.M., Linne, M.A., and Hertzberg, J.R., "Uncertainties associated with the post-processing of 2-D particle Image velocimetry (PIV) velocity data of unsteady flow fields." Paper Number WSS 96S-005, Spring Meeting Western States Section / the Combustion Institute, Tempe, AZ, March, 1996.
- Luff, J.D., Rompage, A.M., Linne, M.A., and Hertzberg, J.R., "Uncertainties associated with the post-processing of (PIV) data." Work-In-Progress Poster 5-017 at the 26th International Symposium on Combustion, Naples, Italy, July 29-August 2, 1996.
- Matalon, M., Flame propagation in closed vessels. *Mathematical Modeling in Combustion Science*, Springer Verlag, pp. 163-175 (1995).
- Matalon, M. "Modelling combustion phenomena." Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland, 1995.
- Matalon, M., "An evolution equation describing the propagation of premixed flames in closed tubes." 48th Annual Meeting of the Division of Fluid Dynamics, American Physical Society, Irvine, CA, 1995.
- Matalon, M., "Near limit oscillations of spherical diffusion flames." 34th Aerospace Sciences Meeting and Exhibit, American Institute of Aeronautics and Astronautics, Reno, Nevada, 1996.
- Matalon, M., "Flame propagation in closed tubes." Sixth International Conference on Numerical Combustion, New Orleans, Louisiana, 1996.
- Mattor, T., and Moore, J.J., "Self-propagating high-temperature synthesis of porous ceramics in microgravity." Experimental Methods for Microgravity Science, Annual TMS Conf., Anaheim, CA, February 4-8th, 1996.

- Mattor, T., and Moore, J.J., "Self-propagating high-temperature synthesis of porous ceramics in microgravity." Experimental Methods for Microgravity Science, Annual TMS Conf., Anaheim, CA, February 4-8th, 1996.
- Mattor, T., and Moore, J.J., "Self-propagating high-temperature synthesis of porous ceramics in microgravity." Amer. Ceram. Soc. Conf., Indianapolis, IN, April 14-17th, 1996.
- McKinnon, J.T., Todd, P.W., and Oberdorster, G. "Combustion of PTFE: The effects of gravity on ultrafine particle combustion." (CASI N96-30806) NASA CR 201112 (June 22, 1996).
- Menon, S., "Parallel simulations of unsteady turbulent flames." Proceedings of the 1996 EUROSIM International Conference HPCN Challenges: Parallel Simulation of Complex Systems and Large-Scale Applications", Delft, The Netherlands, Elsevier Science, to appear, 1996.
- Menon, S. and Chakravarthy, K., "Large-eddy simulations of turbulent premixed flames in couette flow." AIAA 96-3077, 32nd AIAA/ASME/SAE/ASEE Joint Propulsion Meeting, Orlando, FL, July 1-3, 1996.
- Mikami, M., Habara, O., Kono, M., Sato, J., Dietrich, D.L., and Williams, F.A., Pressure effects in droplet combustion of miscible binary fuels. Combustion Science and Technology, (1996).
- Min, S. and Gomez, A. High resolution measurement of single spherical particles using the FFT of the angular scattering intensity. Applied Optics, (August, 1996).
- Molodetsky, E.E., and Dreizen, E.L., "High-temperature oxygen dissolution in liquid zirconium." Presented at the Materials Research Society 1995 Fall Meeting, Boston MA, November 27 to December 1, 1995.
- Molodetsky, I.E. and Dreizen, E.L., "High temperature oxygen dissolution in liquid zirconium." Paper presented at the Fall Meeting, Materials Research Society, Boston MA, November 27, - December 1, 1995.
- Molodetsky, I.E.; Dreizen, E.L.; and Law, C.K. "On the evolution of particle temperature and internal composition for zirconium burning in air." Paper 442, presented at the 26th Symposium (International) on Combustion, The Combustion Inst., Naples Italy, July 29 - August 2, 1996.
- Mueller, C.J., Driscoll, J.F., Reuss, D.L., Drake, M.C., and Rosalik, M.E., Generation and attenuation of vorticity by flames: measured vorticity field time evolution during a premixed flame-vortex interaction. Combustion & Flame, (in print 1996).
- Patnaik, G., Kailasanath, K. and Sinkovits, R., "FLAME3D: a new time-dependent, three-dimensional flame model with detailed chemistry." Paper No. 30, Fall Technical Meeting of the Eastern States Section of the Combustion Institute, Worcester, MA, October 16-18, 1995.
- Patnaik, G., Kailasanath, K., and Sinkovits, R.S., "A new time-dependent, three-dimensional, flame model for laminar flames." Presented at the 26th Symposium (International) on Combustion, Naples, Italy, July 1996.
- Qian, J., and Law, C.K., On the spreading of unsteady cylindrical diffusion flames. Combustion and Flame, (accepted 1996).
- Qian, J., Bechtold, J.K., and Law, C.K., On the response of spherical premixed flames under rotation. Combustion and Flame, (accepted 1996).
- Ramadan, B. and Wichman, I.S., "A numerical study of two-dimensional laminar flames anchored by a dividing plate." Central States Section of the Combustion Institute, 1996.
- Raymond, C.S., and Volpert, V.A., Stability of uniformly propagating SHS waves in porous solids with melting and flow of reactants. Chemical Engineering Science, (accepted 1996).
- Raymond, C.S., and Volpert, V.A., Stabilization of gasless combustion waves by high melting temperature additives. International Journal of SHS, (accepted 1996).
- Ronney, P.D. "Combustion experiments in space." 36th Israel Annual Conference on Aerospace Sciences, Haifa, Israel, February 21-22, 1996.

- Ross, H. "Measurements and predictions of soot formation in laminar premixed flames." Spring Technical Meeting of the Combustion Institute central States Section, St. Louis, MO, May 6, 1996.
- Ross, H. "Soot formation in laminar premixed ethylene/air flames at atmospheric pressure." (Poster presentation) 26th Symposium on Combustion, The Combustion institute, Naples, Italy, July 30, 1996.
- Schult, D.A., Matkowsky, B.J., Volpert, V.A., and Fernandez-Pello, A.C., Propagation and extinction of forced opposed flow smolder waves. *Combustion and Flame*, vol. 101, pp. 471-490 (October 1995).
- Schult, D.A., Matkowsky, B.J., Volpert, V.A., and Fernandez-Pello, A.C., Forced forward smolder combustion. *Combustion and Flame*, vol. 104, pp. 1-26 (1996).
- Shamim, T., and Atreya, A., "Dynamic response of radiating flamelets subject to variable reactant concentrations." presented to the Central States Section Meeting of the Combustion Institute, St. Louis, 1996.
- Shenoy, A.K., Agrawal, A.K. and Gollahalli, S.R., "Visualizing reacting flow computations by rainbow Schlieren imaging." presented at the meeting of the Central States Section of the Combustion Institute, May 5-7, 1996.
- Sheu, J.-C., Numerical Simulation of Burke-Schumann Diffusion Flames Using Finite-Rate Chemical Kinetics, Ph.D. Dissertation. The University of Iowa, Iowa City, Iowa,, (May, 1996.).
- Sheu, J.-C. and Chen, L.-D., A higher-order accurate model for the simulation of time-dependent variable density flow. *AIAA J.*, vol. 34, no. 10, (1996).
- Sheu, J.-C and Chen, L.-D., "A reduced mechanism for prediction of NOx emission from atmospheric methane-air diffusion flame." *Proceedings of the 1996 Spring Technical Meeting of the Central States Section of The Combustion Institute*, St. Louis, MO, pp. 52-57, May 5-7, 1996.
- Sheu, J.-C and Chen, L.-D., "A numerical investigation of the effects of radiative heat transfer on the structure of a gaseous diffusion flame." Paper No. 96-3091, the 1996 AIAA/ASME/ASCE/SAE Joint Propulsion Conference, Lake Buena Vista, FL, 1-3 July, 1996.
- Shkadinsky, K.G., Shkadinskaya, G.V., and Matkowsky, B.J., Gravity induced separation in liquid flames. *Combustion Science and Technology*, (accepted 1996).
- Shkadinsky, K.G., Shkadinskaya, G.V., and Matkowsky, B.J., Gravitational effects on SHS production of high porosity materials. *Combustion Science & Technology*, (accepted 1996).
- Shkadinsky, K.G., Shkadinskaya, G.V., and Volpert, V.A., Stability of liquid flame combustion waves. *Chemical Engineering Science*, (accepted 1996).
- Struk, P. and Tien, J.S., Large droplet combustion and extinction experiment conducted in reduced gravity aboard an aircraft. *Microgravity Science and Technology*, (1996).
- Sung, C.J., and Law, C.K., "Extinction mechanisms of near-limit premixed flames and extended limits of flammability." 26th International Combustion Symposium, Naples Italy, 1996.
- Trees, D., Brown, T.M., Seshadri, K., Smooke, M.D., Balakrishnan, G., Pitz, R.W., Giovangigli, V., and Nandula, S.P., The structure of nonpremixed hydrogen-air flames. *Comb. Sci. and Tech.*, 104, (October 1995).
- VanDerWege, B.A., Bush, M.T., Hochgreb, S., and Linteris, G.T., "Effect of CF3H and CF3Br on laminar diffusion flames in normal and microgravity." Eastern States Section Meeting/The Combustion Institute, Worster, MA, October 1995.
- Wichman, I. S., "Recent theoretical research on diffusion flames and premixed flames with significant heat losses." Sandia Labs invited presentation, May 17, 1996.
- Wichman, I.S.. and Ramadan, B., "Parametric dependencies of lifted and attached diffusion flames near cold walls." Central States Section of the Combustion Institute, 1996.

Winter, M. "In-flight laser induced fluorescence from microgravity droplet combustion." Optical Society of America Topical Meetings Conference, Orlando, FL, March 18-22, 1996.

Winter, M., "In-flight laser diagnostics for microgravity droplet combustion." presented at the 34th Aerospace Sciences Meeting and Exhibit. Reno, NV, Jan. 15-18, 1996.

Winter, M., "In-flight laser diagnostics of microgravity droplet combustion." poster presentation at the Gordon Conference on The Chemistry and Physics of Laser Diagnostics of Combustion, Plymouth, NH, October 1995.

Winter, M., "Laser diagnostic measurements of fundamental processes in droplets." Seminar given at Brown University, Providence, RI, October 31, 1995.

Winter, M. "In-flight laser induced fluorescence from microgravity droplet combustion." presented at the Optical Society of America Topical Meetings Conference. Orlando, FL, March 18-22, 1996.

Yang, J.C., Hamins, A., Gorchkov, N., and Glover, M., "Combustion of polymethylmethacrylate spheres." 26th International Symposium on Combustion 1996.

Yang, J.C., Hamins, A., Gorchkov, N., and Glover, M., "Combustion of polymethylmethacrylate spheres at normal and reduced gravity." Annual Conference on Fire Research, October 28-31, 1996.

Yi, H.-C., Varma, A., Rogachev, A.S., and McGinn, P.J., Gravity-induced microstructural non-uniformities during combustion synthesis of intermetallic-ceramic composite materials. *Ind. Eng. Chem. Research*, vol. 35, pp. 2982-2985 (September 1996).

Zhang, C., Atreya, A., Kim, H.K., Suh, J., and Shamim, T., "The effect of flame structure on soot inception, growth and oxidation in counterflow diffusion flames." presented to the Central States Section Meeting of the Combustion Institute, St. Louis, 1996.

Zhang, C., Atreya, Shamim, T., A., Kim, H.K., and Suh, J., "Measurements of OH, CH, C₂ and PAH in laminar counterflow diffusion flames." presented to the Central States Section Meeting of the Combustion Institute, St. Louis, 1996.

Ground: Fluid Physics

Abdollahian, D., Quintel, J., Zahm, J., and McQuillen, J., Experimental and Analytical Study of Two-Phase Flow Parameters in microgravity. NASA Conference Publication, 3338, pp. 103-108 (1996).

Ackerson, B.J., He, Y. and Davis, K., "Growth and morphology of crystals made of hard spheres." NASA Fluid Physics Conference, NASA Lewis, Cleveland, Ohio, June, 1996.

Ahmed, A.M. and Elghobashi, S.E., Direct numerical simulation of particle dispersion in homogeneous turbulent shear flows. *Journal of Fluid Mechanics*, (July 1996).

Ahmed, S., Carey, V.P., and Motil, B. "Marangoni effects in the boiling of binary fluid mixtures." Third Microgravity Fluid Physics Conference, Cleveland, OH, June 13-15, 1996.

Alexander, J.I.D., "Large deformations of liquid bridges." Invited presentation at The Second Symposium on Fluids in Space, Naples, Italy, April 22-26, 1996.

Alexander, J.I.D., Delafontaine, S., Resnick, A., and Zhang, Y., "Large deformations of liquid bridges." Proceedings of the 2nd Symposium on Fluids in Space, Naples, Italy, April 22-26, 1996.

Alexander, J.I.D., Zhang, Y., Delafontaine, S., and Fedoseyev, A., Numerical simulation of liquid bridge dynamics and statics. *Iz. Mekanika i gaza*, (1996).

Andereck, D.C., "Instabilities in multiple-layer convection." Society of Engineering Science Annual Meeting, Chandrasekhar Memorial Symposium, Tempe, Arizona, October 1996.

- Andereck, D.C., Colovas, P.W., and Degen, M.M., "Observations of time-dependent behavior in the two-layer Rayleigh-Bénard system." Proceedings of the workshop "Analysis of multi-fluid flows and interfacial instabilities," 1996.
- Andereck, D.C., Colovas, P.W., Degen, M.M., "Observations of time-dependent behavior in the two-layer Rayleigh-Bénard system." Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, Ohio, June 13-15, 1996.
- Anderson, D.M. and Davis, S.H., The spreading of volatile liquid drops on heated surfaces. *Physics of Fluids*, vol. 7, pp. 248 (1996).
- Anderson, D.M. and Worster, M.G., Weakly-nonlinear analysis of convection in a mushy layer during the solidification of alloys. *Journal of Fluid Mechanics*, 302, 307-331 (October 1995).
- Anderson, D.M. and Worster, M.G., A new oscillatory instability in a mushy layer during the solidification of binary alloys. *Journal of Fluid Mechanics*, 307, 245-267 (1996).
- Anderson, D.M., Worster, M.G., and Davis, S.H., The case for a dynamic contact angle in containerless solidification. *Journal of Crystal Growth*, vol. 163, pp. 329 (1996).
- Anderson, D.M., Worster, M.G., and Davis, S.H., The case for a dynamic contact angle in containerless solidification. *J. Crystal Growth*, (1996).
- Anderson, D.M., Worster, M.G., and Davis, S.H., Dynamic contact angles in containerless solidification. *Journal of Crystal Growth*, 163/3, 329-338 (1996).
- Anderson, J.L. Electrokinetic Transport of Colloidal Particles with Heterogeneous Surfaces. *J. Electrostatics*, vol. 34, 189 (1995).
- Ashgriz, N., "Dancing bubbles." Department of Mechanical Engineering, University of Victoria, Victoria, CANADA, May 15, 1996.
- Ashgriz, N., "Dancing bubbles." Department of Mechanical Engineering, The University of British Columbia, Vancouver, CANADA, May 16, 1996.
- Ashgriz, N., "Dancing bubbles." Department of Physics, State University of New York at Buffalo, Buffalo, NY, September 10, 1996.
- Avedisian, C.T. and Zhao, Z., "Experimental study of liquid jet impingement in microgravity: the hydraulic jump." 3rd Int. Microgravity Fluid Physics Conf., Cleveland, June 12-14, 1996.
- Avedisian, C.T. and Zhao, Z., "The hydraulic jump in microgravity. *J. Fluid Mech.*, (1996).
- Baker, G. and Koester, G., "Steady-state computations in a vertical Bridgman Furnace." American Physical Society Division of Fluid Dynamics Meeting, Irvine, CA, November 1995.
- Baker, G.R. and Koester, G., "Steady-state computations in a vertical Bridgman furnace." American Physical Society Division of Fluid Dynamics Meeting, Irvine, CA, November 1995.
- Balakotaiah, V. and Jayawardena, S. S., "Stability of wavy films in gas-liquid two-phase flow at normal and microgravity conditions." Proceedings of the 3rd Microgravity Fluid Physics Conference, NASA CP-3338, 1996.
- Balasubramaniam, R. and Subramanian, R.S., Thermocapillary bubble migration - thermal boundary layers for large Marangoni numbers. *Int. J. Multiphase Flow*, vol. 22, no. 3, pp 593 - 612 (1996).
- Banavar, J.R., "Continuum Deductions from Molecular Hydrodynamics." CECAM Conference "The Microscopic Approach to Complexity by Molecular Simulations", Lyon, July 1996.
- Banavar, J.R., "Continuum Deductions from Molecular Hydrodynamics." 6th International Conference on Discrete Models for Fluid Mechanics, Boston (Aug. 1996).

- Barbat, T., Ashgriz, N., "Dancing bubbles and drops." 9th Annual Conference on Liquid Atomization and Spray Systems, San Francisco, CA, May 19-22, 1996.
- Barbat, T., Ashgriz, N., and Lie, C., Interaction between gas bubbles in acoustic pressure fields. *Journal of Fluid Mechanics*, (1996).
- Barbat, T., Ashgriz, N., and Liu, C.S., "Dynamics of two interactive bubbles in an acoustic field - part I: theory." Annual Meeting of the Division of Fluid Dynamics of American Physical Society, Syracuse, New York, November 20-22, 1996.
- Barbat, T., Ashgriz, N., and Liu, C.S., "Dynamics of two interactive bubbles in an acoustic field - part II: experiments." Annual Meeting of the Division of Fluid Dynamics of American Physical Society, Syracuse, New York, November 20-22, 1996.
- Barbat, T., Ashgriz, N., Liu, C.S., "Nonlinear bubble interactions in acoustic pressure fields." Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 13-15, 1996.
- Barchini, R., and Saville, D.A. Dielectric Response Measurements on Concentrated Dispersions. *J. of Colloid & Interface Science*, vol. 176, 86-91 (1995).
- Barchini, R., and Saville, D.A. Electrokinetic Properties Of Surfactant Stabilized Emulsion Droplets. *Langmuir*, vol. 12, 1442-1445 (1996).
- Baygents, J.C., Rivette, N.J., and Stone, H.A. Electrohydrodynamic deformation and interaction of drop pairs in viscous fluids. *J. Fluid Mech.*, accepted, (1996).
- Berg, R.F., "Internal waves in xenon near the critical point." March meeting of the American Physical Society, St. Louis, MO, March 20, 1996.
- Berg, R.F., "Internal waves in CVX." Third Microgravity Fluid Physics Conference, Cleveland, OH, June 14, 1996.
- Berg, R.F., Lyell, M.J., McFadden, G.B., and Rehm, R.G., Internal waves in xenon near the critical point. *Phys. Fluids*, 8, p. 1464 (1996).
- Bernal, L.P. and Maksimovic, P., "Investigation of drop formation by a vortex ring in microgravity." paper presented to The Third Microgravity Fluids Physics Conference, NASA, Cleveland OH, publication 3338, pp 501-508, June 13-15, 1995.
- Bhagavatula, R. and Jasnow, D., Phase asymmetry in thermocapillary motion. *J. Chem. Phys.*, 105, 337 (1996).
- Bousman, W.S., Witte, L.C. and McQuillen, J.B. Gas-liquid flow patterns in microgravity: effects of tube diameter, liquid viscosity and surface tension". *International Journal of Multiphase Flow*, (in press, 1996).
- Brackbill, J.U., and Kothe, D.B., "Dynamical modeling of surface tension." Third Microgravity Fluid Physics Conference, NASA Lewis, Cleveland, June 1996.
- Braunsfurth, M. and Homsy, G.M., "Experimental Study of Buoyant-Thermocapillary Convection in a Rectangular Cavity." Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June, 1996.
- Braunsfurth, M. and Homsy, G.M., Combined thermocapillary-buoyancy convection in a cavity: an experimental study: Part II. *Phys. Fluids*, (1996).
- Braunsfurth, M. and Homsy, G.M., "Combined thermocapillary-buoyancy convection in a in a cavity: an experimental study." American Physical Soc. Meeting, Div. Fluid Dynamics, Irvine CA, November 1995.
- Braunsfurth, M., and Homsy, G.M., "Combined thermocapillary-buoyancy convection in a cavity: an experimental study." Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 1996.
- Brenner, H. and Nadim, A. The Lorentz reciprocal theorem for micropolar fluids. *J. Eng. Math.*, vol. 30, 169-176 (1996).

Brown, J.R. and Hallinan, K.P., Effects of heat induced instabilities on the heat transfer of a stably evaporating meniscus. AIAA, 96-0723, (1996).

Brusstar, M.J., Merte, H., Jr., "The role of buoyancy orientation on bubble residence times and the related critical heat flux." Proc. of Symposium "Heat Transfer in Microgravity Systems," ASME HTD-Vol. 305, pp. 15-27, National Heat Transfer Conf. Portland, OR, Aug. 5-9, 1995.

Brusstar, M.J., Merte, H., Jr., Effects of heater surface orientation on the CHF: Part II. A model for pool and forced convection subcooled boiling. J. Heat Mass Transfer, (1996).

Brusstar, M.J., Merte, H., Jr., Keller, R.B., and Kirby, B.J., Effects of heater surface orientation on the CHF: Part I. An experimental evaluation of models for subcooled pool boiling. Int. J. Heat Mass Transfer, (1996).

Chai, A-T. and Zhang, N., "Marangoni-Benard convection in an evaporating liquid thin layer." The Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 13-15, 1996.

Chang, H-C., Demekhin, E.A., and Kalaidin, E., "Scalings, self-similarity and statistics of interfacial turbulence on a falling film." SIAM conference proceedings, accepted 1996.

Chang, H-C., Demekhin, E.A., Kalaidin, E., and Ye, Y., Scalings of Spatio-temporal Dynamics on a falling film. Physica Scripta, (accepted 1996).

Chang, H-C., Demekhin, E.A., Kalaidin, E., and Ye, Y., Coarsening dynamics of falling film solitary waves. Phys Rev E., (accepted 1996).

Chen, A., Concus, P., Finn, R., and Weislogel, M., On cylindrical container sections for a capillary free-surface experiment. Lawrence Berkeley Lab, Report LBL-36629 Rev., (Nov. 1995).

Chen, C.F., "Particle flux through sediment fingers." Proceedings of the 12th Australasian Fluid Mechanics Conference, Sydney, Australia, pp. 171-174, December 10-15, 1995.

Chen, C.F., "Particle flux through sediment fingers." 48th Annual Meeting of APS - DFD, University of California, Irvine, November 1995.

Chen, C.F. and Chan, C.L., "Salt-Finger convection in a stratified fluid layer induced by thermal and solutal capillary motion." Proceedings of the NASA 3rd Fluid Physics Conf., NASA Lewis Research Center, June 13-15, 1996.

Chen, Y.-J. and Steen, P. H., "Influence of thermocapillary flow on capillary stability: long float-zones in low gravity." Proceedings of the Third Microgravity Fluid Physics Conference, Cleveland OH, June 13-15, 1996.

Chen, Y.-J. and Steen, P.H., Suppression of the capillary instability in the Rayleigh-Taylor slot problem. Phys. Fluids 8, 1, 97-102 (1996).

Chen, Y.-J. and Steen, P. H., "Stabilizing interfaces of finite extent with flow induced by thermal convection, in advances in multi-fluid flows." SIAM publishers, 211-18, 1996.

Chen, Y.-J. and Steen, P. H., "Influence of thermocapillary flow on capillary stability: long float-zones in low gravity." Proceedings of Third Microgravity Fluid Physics Conference, Cleveland OH, June 13-15, 1996.

Chiareli, A.O.P. and Worster, M.G., Flow focusing instability in a solidifying mushy layer. Journal of Fluid Mechanics, 297, 293-305 (October 1995).

Chigier, N. and Humphrey, W., "Transport phenomena in stratified multi-fluid flow in the presence and absence of gravity." Third Microgravity Fluid Physics Conference, 1996.

Chung, J.N., Snyder, T.J., and Sitter, J.S., "Microgravity boiling in an external force field." Proceedings of the 20th International Symposium on Space Technology and Science, held in Gifu, Japan, pp. 195-200, May 19-25, 1996.

Clark, I.O. "Characterization of flows in a horizontal CVD system using laser velocimetry and thermal imaging." Tenth American Conference on Crystal Growth, Vail, CO, August 4-9, 1996.

- Clark, I.O. and Johnson, E.J. "Microgravity particle dynamics." Third Microgravity Fluid Physics Conference, Cleveland, OH, June 13-15, 1996.
- Colin, C., Fabre, J., and McQuillen, J., Bubble and slug flow at microgravity conditions: state of knowledge and open questions. Chemical Engineering Communications, vols 141-142, pp. 155-173 (October 1995).
- Colovas, P.W., Degen, M.M., and Andereck, C.D., Observations of time-dependent behavior in a two-layer Bernard System of rectangular geometry. Bull. Amer. Phys. Soc., vol. 40, (October 1995).
- Concus, P. and Finn, R., Comments on a paper by Keller, King, and Merchant. Nonlinear Anal., (1996).
- Concus, P. and Finn, R., Capillary wedges revisited. SIAM J. Math. Anal., 27, pp. 56-69 (1996).
- Concus, P. and Finn, R., "Equilibrium free-surface configurations: mathematical theory and space experiments." 27th AIAA Fluid Dynamics Conference, New Orleans, Paper AIAA 96-2047, June 1996.
- Concus, P. and Finn, R., "Equilibrium Fluid Interface Behavior Under Low- and Zero-Gravity Conditions." Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 13-15, 1996.
- Concus, P., Finn, R., and Weislogel, M., "Proboscis container shapes for the USML-2 ." Interface Configuration Experiment, in Materials and Fluids Under Low Gravity, L. Ratke, H. Walter, and B. Feuerbacher, eds., Lecture Notes in Physics Vol. 464, Springer-Verlag, Berlin, 1996, pp. 261-270.
- Concus, P., Finn, R., Weislogel, M.M., Interface Configuration Experiments (ICE) Explore the Effects of Microgravity Fluids," Research and Technology (R and T) , . NASA Tech Brief, NASA TM 107111, pg 140 (October, 1995).
- Coriell, S.R., Murray, B.T., Chernov, A.A., and McFadden, G.B., Effects of shear flow and anisotropic kinetics on the morphological stability of a binary alloy. Metallurgical and Materials Trans., 27A, pp. 687-694 (1996).
- Coriell, S. R., Murray, B. T., Chernov, A. A., and McFadden, G. B., "Step bunching on vicinal stepped faces growing from solutions and melts." Tenth American Conference on Crystal Growth, Vail, CO., August 1996.
- Coriell, S.R., Murray, B.T., Chernov, A.A., and McFadden, G.B., "The effect of a shear flow on the morphological stability of a vicinal face: growth from a supersaturated solution." 31st COSPAR Scientific Assembly, Birmingham, England, July 1996.
- d'Ortona, U., DeConinck, J., Koplik, J. and Banavar, J.R., Terraced spreading mechanisms for chain molecules. Phys. Rev., E 53, 562-569 (1996).
- Davis, K.A., Acton, S.T. and Ackerson, B.J., "Segmentation of colloidal crystal images by local histogram analysis." Proceedings of the 1996 Southwest Symposium on Image Analysis and Interpretation Proceedings, pages 178-183, 1996.
- Davis, K.A., Acton, S.T. and Ackerson, B.J., "Segmentation of colloidal crystal images by local histogram analysis." IEEE Southwest Symposium on Image Analysis and Interpretation, San Antonio, Texas, April, 1996.
- Degen, M.M., Colovas, P.W., and Andereck, C.D., Convective flow in two immiscible fluid layers in an annular geometry. Bull. Amer. Phys. Soc., vol. 40, 1955 (October 1996).
- Dell'Aversana, P., Banavar, J.R. and Koplik, J., Suppression of coalescence by shear and temperature gradients. Phys. Fluids 8, 15-28 (1996).
- Dell'Aversana, P., Koplik, J. and Banavar, J.R., Suppression of coalescence by shear and temperature gradients. Phys. Fluids, vol. 8, no. 15, (1996).
- DePaoli, D.W., Basaran, O.A., Feng, J.Q., and Scott, T.C., Forced oscillations of pendant drops. Sep. Sci. Tech., (accepted 1996).
- DePaoli, D.W., Feng, J.Q., Basaran, O.A., and Scott, T.C., Hysteresis in forced oscillations of pendant drops. Phys. Fluids, (accepted 1996).

- Duh, J.C. and S. Yu and B. Jiang, "Three-dimensional simulations of Marangoni-Benard convection by the least-square finite element method." presented at 1996 AIAA Symposium on Microgravity Science, 1996.
- Durian, D., "Foam structure and rheology." University of Illinois at Champagne-Urbana, Dept. of Theor. & App. Mech., 1996.
- Durian, D., "Foam structure and rheology." University of Michigan, Dept. of Physics, 1996.
- Durian, D., "Foam structure and rheology." University of Pennsylvania, Dept. of Physics, 1996.
- Durian, D., "Foam structure and rheology." University of Pittsburgh, Dept. of Physics, 1996.
- Durian, D., "Foam structure and rheology." College de France, 1996.
- Durian, D., "Foam structure and rheology." Universit=E9 de Strasbourg, LUDFC and Institut de Physique, 1996.
- Durian, D., "Foam structure and rheology." Institut Curie, 1996.
- Durian, D.J., Two-stream theory of diffusing-light spectroscopies. *Physica A* , 229, 218-235 (1996).
- Durian, D.J. and Rudnick, J., Photon migration at short times and distances and in cases of strong absorption. *J. Opt. Soc. Am A*, (1996).
- Edwards, B.F., Gray, D.D., and Huang, J., "Magnetothermal convection in nonconducting diamagnetic and paramagnetic fluids." paper presented at the Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 13-15, 1996.
- Elghobashi, S.E. and Lasheras, J., Explosive breakup of a liquid jet by a swirling coaxial gas jet. *Physics of Fluids*, vol. 8, no. 7, p 1696 (July, 1996).
- Erker, J.A. and Baygents, J.C. Electrohydrodynamic interaction of a pair of spherical drops. NASA Conference Publication 3338, 731-735 (1996).
- Esmaceli, A., Arpaci, V.S., Chai, A.T., "Direct numerical simulations of evaporating droplets." Second European Symposium on Fluids in Space, Naples, Italy, 22-26, 1996.
- Faghri, A. and Khurstalev, D., "Evaporation, boiling and condensation on/in capillary structure of high heat flux two-phase devices." Proceedings of the Third Microgravity Fluid Physics Conference, Cleveland OH, June 13-15, 1996.
- Farooq, A. and Homsy, G.M., Linear and nonlinear dynamics of a differentially heated slot under gravity modulation. *J. Fluid Mech.*, vol.313, pp. 1-38 (1996).
- Favier, J.J, Lehmann, P., Drevet, B., Garandet, J.P., Camel, D. and Coriell, S.R., A study of morphological stability during directional solidification of a Sn-Bi alloy in microgravity, in materials and fluids under low gravity. *Lecture Notes in Physics*, ed. L. Ratke, H. Walter, and B. Feuerbacher (Springer-Verlag, Berlin), vol. 464, p. 77-94 (1996).
- Felt, D. W, Hagenbuechle, M., Liu, J., and Richard, J., Experimental study of the rheological behavior of a magnetorheological fluid. *J. Rheology*, (1996).
- Felt, D.W., Hagenbuechle, M., Richard, J., and Liu, J., "Rheology of a magnetorheological fluidand." Proceedings of the 5th Int. Conf. on Electrorheological Fluids, Magnetorheological Suspensions and Associated Technology, p. 738, University of Sheffield, UK, W. Bullough, World Science, 1996.
- Felt, D.W., Hagenbuechle, M., Richard, J., Liu, J. Rheology of a magnetorheological fluidand. *J. Intelligent Systems & Structures*, (September 1996).
- Finn, R., Local and global existence criteria for capillary surfaces in wedge domains. *Calculus of Variations*, 4, pp. 305-322 (1996).
- Finn, R., On a proposition of Lancaster and Siegel. Mathematics Institute, University of Leipzig, (1996).

- Finn, R., "On solutions of mean curvature type inequalities, in Partial Differential Equations and their Applications." P. Marcellini, G. Talenti, and E. Vesentini, eds., Marcel Dekker, pp. 147-154, 1996.
- Finn, R., "Capillary surfaces in wedge domains: new results." World Congress of Nonlinear Analysts, Athens, Greece, July 1996, and Univ. Dresden, Germany, June 1996.
- Finn, R., "Capillary surfaces, theory and experiment, from kitchen sink to NASA Space Shuttle." Univ. Leipzig, Germany, June 1996, and Sonoma State Univ., April 1996.
- Finn, R., "Regularity properties of capillary surfaces." Univ. Bochum, Germany, May 1996.
- Finn, R. and Marek J.M., The modified canonical proboscis. Zeit. Anal. Anwend., 15, pp. 95-108 (1996).
- Fore, L.B. and Witte, L.C., "Two-phase heat transfer in microgravity." invited paper, International Conference on Heat Transfer with Change of Phase, Kielce, Poland, December, 1996.
- Fore, L.B., Bousman, W.S. and Witte, L.C. "Two-phase flow dynamics and heat transfer in microgravity." presented at the Energy Week Conference and Exhibit, Houston, TX, January 1996.
- Fore, L.B., Witte, L.C. and McQuillen, J.B., Heat transfer to annular gas-liquid mixtures at reduced gravity. Journal of Thermophysics and Heat Transfer, vol. 10, no. 4, 633-39 (1996).
- Fore, L.B., Witte, L.C. and McQuillen, J.B., Thermal hydraulics of two phase slug flow under reduced gravity. Int. Journal of Multiphase Flow, (accepted, 1996).
- Fore, L.B., Witte, L.C. and McQuillen, J.B., "Microgravity heat transfer and pressure drop in gas-liquid mixtures: slug and annular flow." presented at the National Heat Transfer Conference, Houston, TX, 1996.
- Fortmeyer, J.M. and Ronney, P.D., "Radiatively-driven flows in gases." 48th Annual Meeting, Division of Fluid Dynamics, American Physical Society, Irvine, CA., November 19-21, 1995.
- Fortmeyer, J.M. and Ronney, P.D., "Studies of radiation-driven and buoyancy-driven Fluid flows and transport." Third International Microgravity Fluids Workshop, NASA LeRC, Cleveland, OH., June 13-15, 1996.
- Foster, M.R., "Boundary-layer theory for a vertical Bridgman device." American Physical Society Division of Fluid Dynamics Meeting, Irvine, CA, November 1995.
- Foster, M.R., "Boundary-layer theory for a vertical Bridgman device." American Physical Society Division of Fluid Dynamics Meeting, Irvine. CA, November 1995.
- Gaitan, D.F., and Holt, R.G. "Observation of mass transport stability and Faraday instability: why stable single bubble sonoluminescence is possible." 3rd joint meeting of the Acoustical Society of America and the Acoustical Society of Japan, Honolulu, HI, 1996.
- Gallagher, C., Leighton, D.T., Chang, H.C., and McCready, M.J., Fundamental processes of atomization in fluid-fluid flows. NASA Conference Publication , 3338, pp. 89-94 (1996).
- Gallagher, C.T., McCready, M.J., and Leighton, D.T., Experimental investigation of a two-layer shearing instability in a cylindrical Couette cell. Phys. Fluids, (accepted 1996).
- Gast, A.P., "Dynamics of ordered and disordered colloidal suspensions." paper presented by A. Gast, American Institute of Chemical Engineers, Miami Beach, Florida , November 1995.
- Gaver, D.P., Halpern, D., Jensen, O.E., and Grotberg, J.B., Fluid-structure interactions of bubble motion through a compliant channel - a model of pulmonary airway reopening. Euromech, London, England, 344, (April 1996).
- Gaver, D.P., Halpern, D.M., Jensen, O.E., and Grotberg, J.B., The steady motion of a semi-infinite bubble through a flexible-walled channel. J. Fluid Mech., 319, 25-65 (1996).

- Gaver, D.P., Perun, M.L., Halpern, D., and Grotberg, J.B. "The influence of airway wall mechanical properties on airway reopening pressures and wall stresses." Biomedical Engineering Society Annual Fall Meeting, Boston, MA, October 1995.
- Gillon, P. and Homsy, G.M., Combined thermocapillary-buoyancy convection in a cavity: an experimental study. *Phys. Fluids*, (1996).
- Ginzburg, V.V., Beale, P.D., and Clark, N.A., Scaling analysis of particle annihilation systems with long range interaction. *Physical Review Letters*, (accepted 1996).
- Gittings, M.R., and Saville, D.A. Electrophoretic Mobility and Dielectric Response Measurements on Electrokinetically Ideal Polystyrene Latex Particles. *Langmuir*, 11798-11800 (1995).
- Glaser, M.A. and Clark, N.A., Statistics of local order in two dimensional liquids: The geometrical defect condensate controls the statistics of local order in a two dimensional liquid. *Science*, (1995).
- Glaser, M.A., Malzbender, R., Clark, N.A. and Walba, D.M., Atomic-detail simulation studies of smectic liquid crystals. *Molecular Simulation*, (1995).
- Goldburg, W. I., "Using homodyne photon correlation spectroscopy to measure velocity differences over varying length scales." Photon Correlation and Scattering Topical Meeting and Tabletop Exhibit, Capri, Italy, August 21-24, 1996.
- Gopal, A.D. and Durian, D.J., Fast thermal dynamics in aqueous foams. *J. Opt. Soc. Am A*, (1996).
- Goree, J. "Dynamics of a Carbon Particle Cloud in a Sputtering Plasma." Workshop on Dusty Plasmas 1995, Wickenburg, Arizona, October 1995.
- Goree, J. "Plasma Dust Crystallization." NASA Fluid Physics Microgravity Conference, Cleveland, Ohio, June 1996.
- Goree, J., and Pieper, J.B. "Experiments with Strongly-Coupled Dusty Plasmas." Workshop on Dusty Plasmas 1995, Wickenburg, Arizona, October 1995.
- Goree, J., and Pieper, J.B. "Experiments with Strongly-Coupled Dusty Plasmas." Gaseous Electronics Conference, Berkeley, California, October 1995.
- Goree, J., and Pieper, J.B. "Experiments with Strongly-Coupled Dusty Plasmas." American Physical Society, March Meeting, St. Louis, Missouri, March 1996.
- Grotberg, J.B. and Howell, P.D., "The propagation of a liquid bridge through an elastic tube and airway reopening." Biological Fluid Mechanics Symposium, ASME Mechanics and Materials Conference, Baltimore, June 1996.
- Gunes, H., Liakopoulos, A., and Sahan, R.A., Low-dimensional description of oscillatory thermal convection: The small Prandtl number limit. *Theoretical and Computational Fluid Dynamics*, (accepted 1996).
- Gunes, H., Sahan, R.A., and Liakopoulos, A., "Low-dimensional representation of transitional buoyancy-driven flow in a vertical channel with discrete heaters." Proceedings of the 1995 National Heat Transfer Conference, vol.1, A. Oretaga and S.P. Mulay eds., ASME HTD-vol. 303, ASME press, pp.125-137, October 1995.
- Gurtin, M., Polignone, D., and Vinals, J., Two-phase binary fluids and immiscible fluids described by an order parameter. *Mathematical Models and Methods in Applied Sciences*, (in press).
- Hagenbuechle, M., Sheaffer, P., and Liu, J., "Static dynamic light scattering of dilute magnetorheological emulsion." Gordon Conference on Macromolecular and Electrolyte Solutions, Ventura, CA, February 11-16, 1996.
- Haj-Hariri, H. and Borhan, A., "Thermocapillary motion of deformable drops in the presence of surface contamination." Proceedings of the 18th Boundary Element Int. Conf., Brago, Portugal, September, 1996.
- Haj-Hariri, H. and Borhan, A., "Time-dependent thermally-driven interfacial flows in multilayered fluid structures." Proceedings of the Third Microgravity Fluid Phys. Conf., NASA Lewis, Cleveland, OH, June 1996.

Halpern, D., Grotberg, J.B., and Jensen, O.E., "Surfactant spreading in a simple long model." American Physical Society, Division of Fluid Dynamics, 49th Annual Meeting, Irvine, CA, November 1995.

He, Q., Hallinan, K.P., "The development of a full field three-dimensional microscale flow measurement technique for application to near contact line flows." presented at the 3rd Microgravity Fluids Conference, Cleveland, OH, June 13-15, 1996.

He, Q., Hallinan, K.P., and Ovrn, B., "3-d full field PIV with pattern recognition applied to thin liquid films." Presented at the Optical Society of America Annual Meeting, Portland, OH, October 1995.

Hegseth, J., and Garcia, L., "A geophysical flow experiment in a compressible critical fluid." Proceedings of the Third Microgravity Fluid Physics Conference, NASA-LeRC, June 13-15, 1996.

Herman, C., "Experimental investigation of pool boiling heat transfer enhancement in the presence of electric fields." presented at the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, Ohio, June 13-15, 1996.

Herman, C., "Experimental investigation of pool boiling heat transfer enhancement in the presence of electric fields." Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, Ohio, June 13-15, 1996.

Holt, R.G., and Gaitan, D.F. "Proceedings of the 3rd Microgravity Fluid Physics Conference, Cleveland, OH, 1996, NASA CP 3338, p. 591." Proceedings of the 3rd Microgravity Fluid Physics.

Holt, R.G., and Gaitan, D.F. "Single Bubble Sonoluminescence: Illuminating anomalous bubble mechanics." 49th meeting of the American Physical Society, Division of Fluid Dynamics, Syracuse, NY, 1996.

Holt, R.G., and Gaitan, F.D. Observation of stability boundaries in the parameter space of single bubble sonoluminescence. Phys. Rev. Lett., (October 1996).

Howell, P., Cassidy, K., Gavriely, N., Glucksberg, M., and Grotber, J.B., "Airway reopening: theoretical and experimental studies." Experimental Biology '96, Washington, D.C., April 1996.

Howell, P.D. and Grotberg, J.B., "The propagation of a liquid bridge through an elastic tube and airway reopening." Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 13-15, 1996.

Hoyle, R. McFadden, G.B. and Davis, S.H. Pattern selection with anisotropy during directional solidification. Transaction of the Royal Society London, (in press).

Hoyle, R., McFadden, G.B., and Davis, S.H., Pattern selection with anisotropy during directional solidification. Phil. Trans. Roy. Soc., (1996).

Hu, H.C. and Kelly, R.E., Stabilization of longitudinal vortex instabilities by means of transverse flow oscillations. J. Phys. Fluids, (1996).

Huang, J., Edwards, B.F., and Gray, D.D., "Thermoconvective instability of paramagnetic fluids in a uniform magnetic field." abstract presented to the Annual Meeting of the Division of Fluid Dynamics, American Physical Society, 1996.

Huang, W. and Maldarelli, C., The effect of surfactant on the motion of bubbles and drops. CISM Lecture Notes, (1996).

Humphries, Jr., W.M, Bartram, S.M., and Clark, I.O. "Velocity field measurements in a chemical vapor deposition reactor using digital particle image velocimetry." 1996 ASME Symp Laser Anemometry and Experimental and Numerical Flow Visualization, San Diego, CA, July 7-11, 1996.

Huntley, D.A. and Davis, S.H., Oscillatory and cellular mode coupling in rapid directional solidification. Phys. Rev. B , (1996).

Jacqmin, D., "An energy approach to the continuum surface tension method: application to droplet coalescences and droplet/wall interactions." Proceedings of the 1995 ASME IMECE, November 1995.

Jacqmin, D., "An energy approach to the continuum surface tension method." AIAA 96-0858, AIAA 34th Aerospace Sciences Meeting and Exhibit, 1996.

- James, A., Smith, M.K., and Glezer, A. "The explosive ejection of small droplets from a liquid-gas interface." American Physical Society, Division of Fluid Dynamics, November 24-26, 1996.
- Jasnow, D. and Vinals, J., Coarse-grained description of thermocapillary flow. *Phys. Fluids* 8, 600, (1996).
- Jayawardena, S.S., "Two-phase flow at a pipe junction - slug flow." AIChE Annual Meeting, Miami Beach, FL. November 1995.
- Jayawardena, S.S., "Reduced gravity two-phase flow at a tee-junction." Proceedings of the 31st National Heat Transfer conference, Houston, TX, August 1996.
- Jayawardena S.S. and McQuillen, J.B. "Microgravity two-phase flow at a pipe junction." paper 96-2070 presented at the 27th AIAA Fluid Dynamics Conference, New Orleans, LA., June, 1996.
- Jiang, H.D., Kam, V., Kamotani, Y. and Ostrach S., Transport phenomena in supercritical fluid extraction. *Chem. Eng. Comm.*, vol. 132, (October 1995).
- Jiang, H.D., Ostrach, S., and Kamotani, Y., Thermosolutal transport phenomena in large lewis number electrochemical systems. *International Journal of Heat and Mass Transfer*, (1996).
- Jiang, L., Perlin, M., and Schultz, W.W., Breaking faraday waves. 21st ONR Sym of Naval Hydro, Trondheim, NOR, (1996).
- Jiang, L., Ting, C.-L., Perlin, M., and Schultz, W.W., Moderate and steep Faraday waves: instabilities, modulation and temporal asymmetries. *Journal of Fluid Mechanics*, (1996).
- Jieyong, X. and Zebib, A., "Oscillatory thermocapillary convection." Third Microgravity Fluid Physics Conference, Cleveland, OH, June, 1996.
- Jin, Y Y., and Chen, C. F., Stability of convection and heat transfer of high Prandtl number fluids in a vertical slot. *J. Heat Transfer*, vol.118, pp. 359-365 (1996).
- Jin, Y.Y., and Chen, C.F., Natural convection of high Prandtl number fluids with variable viscosity in a vertical slot. *Int. J. Heat Mass Transfer*, vol. 39, pp. 2663-2670 (1996).
- Jin, Y.Y. and Chen, C.F., Effect of gravity modulation on natural convection in a vertical slot. *Int. J. Heat Mass Transfer*, (May 1996).
- Johnson, E.J., Hyer, P.V., Culotta, P.W., and I.O. Clark, I.O. Evaluation of infrared thermography as a diagnostic tool in CVD applications. *J. Crystal Growth*, submitted, (1996).
- Juric, D. and Tryggvason, G., "Direct numerical simulations of flows with phase change." AIAA 96 0857, 34th AIAA Aerospace Sciences Meeting, 1996.
- Juric, D. and Tryggvason, G., "Computations of fluid boiling, in advances in numerical modeling of free surface and interface fluid dynamics." FED-vol. 238, ASME, pp. 341-347, 1996.
- Kang, S.-Y., Sangani, A. S., Tsao, H.-K., and Koch, D.L., Rheology of dense bubble suspensions. *Phys. Fluids*, (1996).
- Kao, S-H, Arpaci, V.S., and Chai, A-T., "Thermocapillary driven flow past marangoni instability." Second European Symposium on Fluids in Space, Naples, Italy, 22-26, 1996.
- Karhikeyan, M., Huang, J., Plawsky, J., and Wayner, P.C., Jr., "Initial nonisothermal experimental study of the constrained vapor bubble thermosyphon." Proceedings of the ASME 31st National Heat Transfer Conference (vol. 5) pp 121-129, ASME, NY, NY, 1996.
- Karhikeyan, M., Huang, J., Plawsky, J., and Wayner, P.C., Jr., "Initial nonisothermal experimental study of the constrained vapor bubble thermosyphon." Paper presented at the National Heat Transfer Conference, Houston, TX, August 3-6, 1996.

- Karthikeyan, M., Huang, J., Plawsky, J.L., and Wayner, P.C., Jr., "Experimental study of the constrained vapor bubble thermosyphon." Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 13-15, 1996.
- Kassemi, M. and Rashidnia, N., "Thermocapillary and natural convective flows generated by a bubble in 1-g and low-g environments." AIAA 34th Aerospace Sciences Meeting and Exhibit, Reno NV, AIAA 96-0734, January 1996.
- Kassemi, M., Rashidnia, N., and Mercer, C., "Low-g and 1g velocity and temperature fields in the vicinity of a bubble on a heated surface." The Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, Ohio, June 1996.
- Koblinski, P., Kumar, S.K., Maritan, A., Koplik, J., and Banavar, J.R., "Interfacial Roughening Induced by Phase Separation." *Phys. Rev. Lett.* 76, 1106-1109 (1996).
- Kim, J. and Kalkur, T.S., "Development of a surface array of microscale heaters to measure wall heat transfer underneath single bubbles in nucleate pool boiling." *Proceedings of the ASME Winter Annual Meeting*, San Francisco, CA, November 1995.
- Kim, J., and Kalkur, T.S., "A surface mounted array of microscale heaters for use in nucleate boiling." presented at the 1995 National Heat Transfer Conference, Portland, OR, August 1995.
- Kim, J., Ch'ng, C.P., and Kalkur, T.S., "Design of an improved heater array to measure microscale wall heat transfer." NASA Conference Publication, 3338, pp. 165-170 (1996).
- Kirk, K., Merte, H. Jr., and Keller, R.B., "Low velocity nucleate flow boiling at various orientations." *J. of Heat Transfer*, 117, 2, pp. 380-386 (October 1995).
- Kizito, J. P., Ostrach, S., and Kamotani, Y., "Free coating flow at high capillary and Reynolds numbers." Ph.D. Thesis, Case Western Reserve University, Cleveland, 1995.
- Koplik, J., "Fluid flow at the molecular scale." Yale University, Mechanical Engineering Dept., November 1995.
- Koplik, J., "Molecular Dynamics of Fluid Flow." Ohio State University, April 1996.
- Koplik, J., "Molecular dynamics of fluid flow." Yale University, November 1995.
- Koplik, J., "Molecular dynamics of fluid flow." Hunter College, February 1996.
- Koplik, J., "Molecular dynamics of fluid flow." Brown University, April 1996.
- Koplik, J., "Molecular dynamics of fluid flow." Third NASA Fluids Conference, Cleveland (June 1996).
- Koplik, J., "Molecular dynamics of fluid flow." Universite de Paris - Orsay, June 1996.
- Koplik, J. and Banavar, J.R., "Corner flow in the sliding plate problem." *Phys. Fluids* 7, 3118-3125 (1996).
- Koplik, J. and Levine, H., "Scattering of superfluid vortex rings." *Phys. Rev. Lett.* 76, 4745-4748 (1996).
- Kothe, D.B., Rider, W.J., Mosso, S.J., Brock, J.S., and Hochstein, J.I., "Volume hacking of interfaces having surface tension in two and three dimensions." 34th Aerospace Sciences Meeting & Exhibit, AIAA, Reno NV, AIAA 96-0859, 1996.
- Kunka, M.D., Tanveer, S., and Foster, M.R., "Nonlinear evolution of the zero surface tension, small Peclet number dendrites." American Physical Society Division of Fluid Dynamics Meeting, Irvine, CA, November, 1995.
- Kunka, M.D., Tanveer, S., and Foster, M.R., "Nonlinear evolution of the zero surface tension, small Peclet number dendrites." American Physical Society Division of Fluid Dynamics Meeting, Irvine, CA., November 1995.
- Kuru, W.C., Sangalli, M., and McCready, M.J., "Transition to Three-dimensional Waves in Cocurrent Gas-liquid Flows." SIAM conference proceedings, accepted 1996.

- Kuru, W.C., Sangalli, M., and McCreedy, M.J., "Onset of transverse in cocurrent gas-liquid flow." AIChE Annual Meeting, October 1995.
- Kuru, W.C., Sangalli, M., Uphold, D.D., and McCreedy, M.J., Linear stability of stratified channel flow. *Int. J. Mult. Flow*, 21, pp 733-753 (October 1995).
- Langbein, D. and Weislogel, M., "Dynamics of liquids in edges and corners (DYLCO)." IML-2 Investigators Annual Meeting, ESRIN, Frascati, Italy, Nov. 7-8, 1995.
- Langbein, D. and Weislogel, M.M., "Dynamics of liquids in edges and corners." 2nd European Symposium Fluids in Space, Naples, Italy, April, 1996.
- Li, W. and Davis, E.J., The effects of gas and particle properties on thermophoresis. *J. Aerosol Sci.* (1995).
- Liakopoulos, A., "Low-dimensional dynamical models of thermal convection." Third Microgravity Fluid Physics Conference, Cleveland, OH, NASA CP 3338, pp 325-330, June 13-15, 1996.
- Liakopoulos, A., "Low-dimensional models of transitional thermal convection." Cornell University, Ithaca, N.Y., October 22, 1996.
- Liakopoulos, A., "Low-dimensional models of transitional flows." University of Maryland, College Park, MD., April 26, 1996.
- Liakopoulos, A. and Blythe, P.A., "Low-dimensional dynamical models of transitional convective flows." APS Meeting, Irvine, CA, November 19-21, 1995.
- Liakopoulos, A. and Blythe, P.A., Low-dimensional dynamical models of transitional convective flows. *Bull. Am. Phys. Soc.*, vol. 40, no. 12, p. 1955 (October 1995).
- Lin, S.P. Regimes of jet breakup and breakup mechanisms. AIAA Progress Series, Recent Advances in Spray Combustion, (1996).
- Lin, S.P. and Friedman, M. Non-equilibrium evaporation from a heated liquid layer. *J. of Thermophysics and Heat Transfer*, vol. 10, 497-503 (1996).
- Liu, J., "Recent development and research in electrorheological and magnetorheological fluids." Complex Fluid Workshop, Chinese Science Academy, September 23-27, 1996.
- Liu, J., "Structure and dynamics of a ferrofluid emulsion in a magnetic field." Symposium on Complex Liquid American Physics Society, St. Louis, March 1996.
- Liu, J., "Static and dynamic properties of chain formation in a dilute magnetorheological fluid." Symposium on Microgravity Science, Sixth International Space Conference of Pacific-Basin Societies, December 6-8, 1995.
- Liu, J., "Field-induced phase transition and structures of ferrofluid emulsions." Seminar, Dept. of Chemistry, UCLA, November 17, 1995.
- Liu, J. and Hagenbuechle, M., "Chain dynamics in a dilute magnetorheological fluid." Proceeding of the Third Microgravity Fluid Physics Conference, NASA Lewis Research Center, Cleveland, OH, June 13-15, 1996.
- Liu, J. and Hagenbuechle, M., "Static light scattering study of chain formation in a dilute ferrofluid emulsion." American Physics Society March Meeting, St. Louis, March 1996.
- Liu, J. and Hagenbuechle, M., "Experimental study of chain formation and chain dynamics in a dilute ferrofluid emulsion." American Physics Society March Meeting, St. Louis, March 1996.
- Liu, J., and Hagenbuechle, M., "Chain dynamics in a dilute magnetorheological fluid." Proceedings of NASA 3rd Microgravity Fluid Physics Conf., Cleveland, OH, June 13-15, 1996.

- Liu, J., Hagenbuechle, M., Sheaffer, P., and Zhu, Y., "Static and dynamic properties of chain formation in a dilute magnetorheological fluid." *Advances in the Astronautical Sciences* (6th ISCOPS), Vol. 91, 431, 1996.
- Loewenberg, M. and Davis, R.H., Near-contact electrophoretic particle motion. *J. Fluid Mech.*, 288, 103-122 (1995).
- Loewenberg, M. and Hinch, E.J. "Self-diffusion of drops in a dilute sheared emulsion." *Third Microgravity Fluid Physics Conference*, NASA Conference Publication 3338, pp. 579-584, 1996.
- Lowry, B.J., and Steen, P.H., Shape stability of slender liquid bridges in axial flows. *J. Fluid Mech.*, (accepted 1996).
- Lyubimov, D., Lyubimov, T., Alexander, J.I.D., and Lobov, N.I., On the Boussinesq approximation for fluid systems with deformable boundaries. *Journal of Fluid Mechanics*, (1996).
- Madanshetty, S.I., Nadim, A., and Stone, H.A. Experimental measurements of shear-induced diffusion in suspension using long time data. *Phys. Fluids*, vol. 8, 2011-2018 (1996).
- Mariarty, J.A. and Grotberg, J.B. "A model of flow-induced instabilities of mucus." *American Physical Society, Division of Fluids Dynamics*, 48th Annual Meeting, Irvine, CA, November 1995.
- Marr-Lyon, M.J., Thiessen, D.B., Marston, P.L., Active acoustic stabilization of capillary bridges significantly beyond the Rayleigh limit: experimental confirmation. *Journal of the Acoustical Society of America*, 99, 2540 (1996).
- Marston, P.L., Capillary bridge stability in an acoustic standing wave: linearized analysis of passive stabilization with radiation pressure. *Bulletin of the American Physical Society*, 40, 1923 (October 1995).
- Marston, P.L., Marr-Lyon, M.J., Morse, S.F., and Thiessen, D.B., "Stabilization and low-frequency oscillation of capillary bridges with modulated acoustic radiation pressure." *Third Microgravity Fluid Physics NASA LeRC Conference*, June 13-15, 1996.
- Martin, B. "Two-dimensional Thermal Convections in Liquid Films." *American Physical Society, Fluid Dynamics Division Annual Meeting*, Irvine, California, November 1995.
- Martin, B., and Wu, X-I. Shear Flow in a Two-dimensional Couette Cell - A Technique for Measuring the Viscosity of Free-standing Liquid Films. *Rev. Sci. Instr.*, vol. 66, 5603 (1995).
- Martin, B., Tharrington, A., and Wu, X-I. Chiral Symmetry Breaking in Crystal Growth: Is Hydrodynamic Convection Relevant? *Phys. Rev. Lett.*, vol. 77, 2826 (1996).
- Maruvada, S.R.K. and Park, C.-C., Retarded motion of bubbles in Hele-Shaw cells. *Phys. Fluids*, (1996).
- Maruvada, S.R.K and Park, C-W., "Retarded motion of bubbles and drops in Hele-Shaw cells." *Annual meeting of AIChE*, Miami, FL, November 1995.
- Maruvada, S.R.K and Park, C-W., "Retarded motion of bubbles and drops in Hele-Shaw cells ." *48th Annual meeting of the Division of Fluid Dynamics*, American Physical Society, Irvine, CA, November 1995.
- McCready, M., "Nonlinear stabilization of interfacial waves in fluid-fluid flows." *Chemical Engineering Department*, Northwestern University, May 30, 1996.
- McCready, M.J., and Chang, H.-C., Formation of large disturbances on sheared and falling liquid films. *Chem. Eng. Comm.*, 141-142, pp 347-358 (1996).
- McCuan, J., Symmetry by spherical reflection and spanning drops in a wedge. *Pacific J. Math*, (in press, 1996).
- Melands, F., and Goree, J. Particle Simulation of Two-Dimensional Dust Crystal Formation. *J. of Vacuum Science and Tech. A*, vol. 14, 519- 524 (1996).
- Melandso, F., and Goree, J. Polarized Supersonic Plasma Flow Simulation for Charged Bodies such as Dust Particles and Spacecraft. *Physical Review E*, vol. 52, 5312-5326 (1995).

- Mercer, C.R., Rashidnia, N., and Creath, K., High data density measurement of quasi-steady-state flows. *EXP. FLUIDS*, 21, (1996).
- Mitus, A.C., Smolej, F., and Patashinski, A.Z. Q446 <Shape Spectroscopy> of local f.c.c. structures in computer simulations of crystallization. *Europhysics Letters*, vol. 32 (9), 777 (December 20, 1995).
- Mo, G., Sangani, A.S., Tsao, H.-K., and Koch, D.L., "Simple shear flows of dense gas-solid suspensions at finite Stokes numbers." Annual Meeting of American Institute of Chemical Engineers, Miami, FL., October 1995.
- Molloy, R.F., Gallagher, C.T., and Leighton, D.T. "Binary Oscillatory Crossflow Electrophoresis." Proceedings of the Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 13-15, 1996.
- Moriarty, J.A. and Grotberg, J.B., Flow induced instabilities of a mucus-serous bilayer. *Euromech*, London, England, 344, (April 1996).
- Moriarty, J.A. and Grotberg, J.B., "A model of flow-induced instabilities of mucus." American Physical Society, Division of Fluid Dynamics, 48th Annual Meeting, Irvine, CA, November, 1995.
- Moriarty, J.A. and Grotberg, J.B., "A model of flow-induced instabilities of mucus." Biomedical Engineering Society Annual Fall Meeting, Boston, MA, October 1995.
- Morse, S.F., Thiessen, D.B., and Marston, P.L. Capillary bridge modes driven with modulated ultrasonic radiation pressure. *Physics of Fluids*, 8, 3-5 (1996).
- Mosler, A.B. and Shaqfeh, E.S.G., The conformation of model polymers in stochastic flow fields: Flow through fixed beds. *Phys. Fluids*, (June 1996).
- Mundrane, M. and Zebib, A., Low Prandtl number Marangoni convection with a deforming interface. *AIAA Journal of Thermophysics & Heat Transfer*, 9, p 795-797 (November 1995).
- Murray, B.T., "The phase-field equations as a computational technique in crystal growth." Tenth American Conference on Crystal Growth, Vail, CO., August 1996.
- Muzny, C.D., Clark, N.A., and Gun Won J., Quenching the Kosterlitz-Thouless transition in two dimensional freely suspended liquid crystal films. *Physical Review Letters*, (accepted 1996).
- Nadim, A. A concise introduction to surface rheology with application to dilute emulsions of viscous drops. *Chem. Eng. Comm.*, vol. 148, 391-407 (1996).
- Nadim, A. "The role of surfactants and surface rheology in determining the rheological properties of dilute emulsions." EuroConference on Constitutive Relations and their Applications, Isaac Newton Institute for Mathematical Sciences, University of Cambridge, Cambridge, UK, April, 1996.
- Nadim, A. "Shape oscillations of gas bubbles with Newtonian interfacial properties." Third Microgravity Fluid Physics Conference, NASA Lewis Research Center, Cleveland, OH, June, 1996.
- Nadim, A. "Constitutive equations for dilute emulsions of viscous drops with interfacial rheology." Sixth International Conference on Discrete Methods in Fluid Mechanics, Boston University, Boston, MA, August 1996.
- Nadim, A., Borhan, A., and Haj-Hariri, H., Tangential stress and Marangoni effects at a fluid-fluid interface in a Hele-Shaw cell. *J. Coll. Interface Sci.*, vol. 181, pp. 159 - 164 (1996).
- Nadim, A., Borhan, A., and Haj-Hariri, H. Tangential stress and Marangoni effects at a fluid-fluid interface in a Hele-Shaw cell. *J. Colloid Interface Sci.*, vol. 181, 159-264 (1996).
- Nakagawa, M., Waggoner, R.A. and Fukushima, E., "NMRI measurements of flow of granular mixtures." Third Microgravity Fluid Physics Conference, Sheraton Cleveland City Center Hotel, NASA LeRC, June 13-15, 1996.
- Narayanan, T., Ye, X., Tong, P., and Huang, J.S., "A neutron scattering study of depletion interactions in a colloid-polymer mixture." American Physical Society March Meeting, St. Louis, March 18-22, 1996.

- Neitzel, G.P. and Riley, J. "Control of oscillatory thermocapillary convection." Symposium on Fluids in Space, Naples, Italy, 1996.
- Nilsen, S.J., "Structure and dynamics in ordered and disordered colloidal suspensions." Dissertation, Stanford University, March 1996.
- Nobari, M.R.H. and Tryggvason, G., Numerical simulations of three-dimensional drop collisions. *AIAA Journal*, 34, pp. 750-755 (1996).
- Nobari, M.R., Jan, Y.-J., and Tryggvason, G., Head-on collision of drops--a numerical investigation. *Phys. Fluids*, 8, pp. 29-42 (1996).
- Oguz, H.N., Takagi, S., and Misawa, M., "Production of gas bubbles in reduced gravity environments." Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 13-15, 1996.
- Oguz, H.N., Takagi, S., and Misawa, M., "Production of gas bubbles in reduced gravity environments." Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 13-15, 1996.
- Ohlsen, D. R., Hart, J. E., and Weidman, P. D., "Waves in radial gravity using magnetic fluid." Third Microgravity Fluid Physics Conference, NASA Lewis Research Center, Cleveland, OH, June, 1996..
- Okumoto, S., Hagenbuechle, M., Liu, J., "Diffusing wave spectroscopy study of dipole dipole interacting Brownian particles." American Physics Society March Meeting, St. Louis, March 1996.
- Or, A.C., Finite wavelength instability in a horizontal liquid layer on an oscillating plane. *J. Fluid Mech.*, (1996).
- Or, A.C., Finite wavelength instability in a horizontal liquid layer on an oscillating plane. *J. Fluid Mechanics*, (1996).
- Or, A.C. and Kelly, R.E., Onset of Marangoni convection in a layer of fluid modulated by a weak nonplanar oscillatory shear. *Ins. J. Heat Mass Transfer*, vol. 38, pp 2269-2280 (October 1995).
- Or, A.C. and Kelly R.E., Finite wavelength instability of a free surface due to an oscillatory shear. *Bull. Am. Phvs. Soc.*, vol. 40, p 1949 (October 1995).
- Oron, A., Deissler, R., and Duh, J.C., Marangoni convection in a layer with two free surfaces. *European Journal of Mechanics, B/Fluids*, vol.6, pp. 737-760 (November 1995).
- Ostrach, S., Kamotani, Y., "Industrial processes influenced by gravity." Third Microgravity Fluids Physics Conference, June 13-15, 1996.
- Pan, R., Green, J. and Maldarelli, C., Measurement of kinetic rate constants for a homologous series of polyethoxylated surfactants. *Langmuir*, (1996).
- Pan, R., Green, J., Pollard, M. and Maldarelli, C., New kinetic and state equations for the adsorption of surfactant on an air/water interface, and measurements of state equation parameters for a homologous series of polyethoxylated surfactants. *J. Colloid and Interface Science*, (1996).
- Pang, J. and Clark, N.A., Dynamics of layer steps in freely suspended liquid crystal films. *Bulletin of the American Physical Society*, 40,85 (October 1995).
- Papadopoulos, D.H. and Rosner, D.E., Enclosure gas flows driven by non-isothermal walls. *Physics of Fluids*, vol. 7, no. 11, pp. 2535-2537 (November, 1995).
- Papadopoulos, D.H. and Rosner, D.E., "Fluid creep effects on near-wall solute transport for non-isothermal ampoules." Proceedings of the Third Microgravity Fluid Physics Conference at NASA LeRC, Cleveland, Ohio, June 13-15, 1996.
- Patashinski, A.Z., One temperature step away from the critical point. *Physical Review E*, vol. 54 (3), p. 2479 (September 1, 1996).

- Patashinski, A.Z., Rapid temperature changes near a critical point. *Physics Letters A*, vol. 219 (1/2), p. 131 (August 12, 1996).
- Patashinski, A.Z. and Ratner, M.A., Orientation relaxation in glassy polymers. II. Dipole-size spectroscopy and short-time kinetics. *The Journal of Chemical Physics*, vol. 103 (24), (December 22 1995).
- Pieper, J.B., Goree, J., and Quinn, R.A. Experimental Studies of 2D and 3D Structure in a Crystallized Dusty Plasma. *J. of Vacuum Science and Tech. A*, vol. 14, 511- 518 (1996).
- Pinarbasi, A. and Liakopoulos, A., On the influence of temperature and viscosity fluctuations on interfacial instability. *Int. Comm. in Heat and Mass Transfer*, vol. 23, pp. 485-493 (November 4, 1996).
- Pinarbasi, A. and Liakopoulos, A., The role of variable viscosity in the stability of channel flow. *International Communications in Heat and Mass Transfer*, vol. 22, no. 6, pp. 837-847 (October 1995).
- Poulikakos, D., Megaridis, C. M. and Vedha-Nayagam, M., "Fluid dynamics and solidification of molten solder droplets impacting on a substrate in microgravity." Presented at the Third Microgravity Fluid Physics Conference, Cleveland OH, June 13-15, 1996.
- Praburam, G., and Goree, J. Sensitivity of the Scattering Ratio Method for Sizing Sub-Micron Particles Suspended in a Plasma. *Plasma Sources Science and Tech.*, vol. 5, 84-92 (1996).
- Praburam, G., and Goree, J. Evolution of a Particulate Cloud in an RF Plasma. *IEEE Transactions on Plasma Science*, vol. 24, 97-98 (1996).
- Praburam, G., and Goree, J. Experimental Observation of Very Low-Frequency Macroscopic Modes in a Dusty Plasma. *Physics of Plasmas*, vol. 3, 1212-1219 (1996).
- Prat, D.M. and Hallinan, K.P., "The effects of near contact line thermocapillary stresses on the wetting characteristics of a heated, evaporating meniscus within a capillary pore." Presented at the National Heat Transfer Conference, Houston, TX, August 5-9, 1996.
- Prosperetti, A. and Oguz, H.N., "Acoustic behavior of vapor bubbles." *Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 13-15, 1996.*
- Quinn, R.A., Cui, C.S., Goree, J., Pieper, J.B., Thomas, H., and Morfill, G. Structural Analysis of a Coulomb Lattice in a Dusty Plasma. *Physical Review E*, vol. 53, 53-56 (1996).
- Rashidnia, N., "Instabilities around a bubble due to combined Marangoni and Buoyancy Effects." *Proceedings of the AIChE Symposium Series*, published paper, vol. 92, no. 310, pp. 110-118, 1996.
- Rashidnia, N., Kassemi, M., and Mercer, C., "Instabilities around a bubble due to combined Marangoni and buoyancy effects." *ASME National Heat Transfer Conference, Houston, Texas, August 1996.*
- Reyes, R., and Wayner, P.C., Jr. "Thin film profile of an extended meniscus in a glass cuvette." Material concerning water presented at the 1995 Annual Meeting of A.I.Ch.E., Miami Beach, FL, November 15-18, 1995.
- Rivette, N.J. and Baygents, J.C. A note on the electrostatic force and torque acting on an isolated body in an electric field. *Chem Eng. Sci.*, vol. 51, 5205-5211 (1996).
- Rogers, C.B. and Squires, K.M., "Decoupling the role of inertia and gravity on particle dispersion." *Microgravity Meeting*, 1996.
- Rosner, D.E. and Papadopoulos, D.H., Jump, creep and slip boundary conditions at non-equilibrium fluid/solid interfaces. *Ind./Eng. Chem. Research*, (September 1996).
- Rush, B.M., Nadim, A., and Azuma, H. "Nonlinear oscillations of two-dimensional drops." *American Physical Society, Division of Fluid Dynamics, Annual Meeting, Syracuse, NY, 1996.*

- Rutgers, M.A, Wu, X-l., Bhagavatula, R., Petersen, A.A., and Goldburg, W.I., Two-dimensional velocity profiles and laminar boundary layers in flowing soap films. *Phys. Fluids*, (in press).
- Sadhal, S.S. "Acoustically levitated drops." Invited lecture, Gotas, burbuja y peliculas (Drops, bubbles & films), Escuela de Fisico-Quimica de Fluidos, Universidad Internacional Menendez Pelayo, Santander, Spain, September 9-13, 1996.
- Sadhal, S.S., Gopinath, A., Oosthuisen, P.H., and Hashemi, A. "Proc. 30th National Heat Transfer Conference - 1995, Vol. 3, "Heat Transfer in Microgravity Systems." Edited by: HTD-Vol. 305, ISBN 0-7918-1704-0 ASME, New York, Vol.3, pp 193, 1995.
- Sahan, R.A., Gunes, H., and Liakopoulos, A., "Low-dimensional models for coupled momentum and energy transport problems." in *Cooling and Thermal Design of Electronic Systems*, C.H. Amon, ed., HTD-vol.319/EEP-vol.15, 1995 International Mechanical Engineering Congress, pp. 1-15, October 1995.
- Sahan, R.A., Liakopoulos, A., Gunes, H., Reduced dynamical models of nonisothermal grooved channel flow. *Physics of Fluids*, (accepted 1996).
- Sangalli, M., Gallagher, C.T., Leighton, D.T., Chang, H.-C. and McCready, M.J., Finite amplitude wave evolution at the interface between two viscous fluids. *Phys. Rev. Lett.*, 75, pp 77-80 (October 1995).
- Sangani, A.S., and Koch, D.L., "Rapidly sheared bubble suspensions." Third Microgravity Fluid Physics Conference, NASA Lewis Research Center, Cleveland, OH, June, 1996.
- Sangani, A.S., Mo G., Tsao, H.-K., and Koch, D.L., Simple shear flows of gas-solid suspensions at finite stokes numbers. *J. Fluid Mech.*, 313, pp. 309-341 (1996).
- Saville, D.A., Trau, M., and Aksay, I.A. "Electrohydrodynamics of aqueous colloidal dispersions: particle deposition and assembly on surfaces." American Institute of Chemical Engineers, 1995 Annual Meeting, Miami, Florida, November 1995.
- Saville, D.A., Trau, M., and Aksay, I.A. "Field-induced two and three-dimensional colloidal crystals." 1995 Materials Research Society Meeting, Boston, Massachusetts, November 1995.
- Schatz, M.F., VanHook, S.J., McCormick, W.D., Swift, J.B., and Swinney, H.L., Onset of surface-tension-driven Benard convection. *Phys. Rev. Lett.*, 75, 1938-1941 (October 1995).
- Schatz, M.F., VanHook, S.J., McCormick, W.D., Swift, J.B., and Swinney, H.L., "Experimental control of thermocapillary convection in a liquid bridge." Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, 1996.
- Schatz, M.F., VanHook, S.J., McCormick, W.D. Swift, J.B., and Swinney, H.L., "Experimental control of thermocapillary convection in a liquid bridge." Proceedings of the Third Microgravity Fluid Physics Conference 1996.
- Schulze, P. and Davis, S.H., Shear stabilization of a solidifying front: Weakly nonlinear analysis in the long-wave limit. (1996).
- Schulze, T.P. and Davis, S.H. The influence of oscillatory and steady shears on interfacial stability during directional solidification. *Journal of Crystal Growth*, vol. 143, pp 317 (1995).
- Schulze, T.P. and Davis, S.H., Shear stabilization of morphological instability during directional solidification. *Journal of Crystal Growth*, vol. 149, pp. 149 (1995).
- Schulze, T.P. and Davis, S.H. Shear stabilization of a solidifying front: Weakly nonlinear analysis in the long wave limit. *Physics of Fluids*, (in press).
- Schulze, T.P. and Davis, S.H. Effects of flow on morphological stability during directional solidification. *Metallurgical and Materials Transactions*, (in press).
- Schulze, T.P., and Davis, S.H., Effects of flow on morphological stability during directional solidification. *Mat. Mater. Trans.*, (1996).

- Schulze, T.P., and Davis, S.H., "Long-wave weakly nonlinear theory for a directionally solidifying binary alloy in the presence of a time-periodic shear flow." Annual Meeting of the Division of Fluid Dynamics, American Physical Society, Irvine, October, 1995.
- Schwartz, L.W., Simulation of droplet motion on heterogeneous surfaces. *Physics of Fluids*, (1996).
- Sekerka, R.F., Coriell, S.R., and McFadden, G.B., Stagnant film model of the effect of natural convection on the dendrite operating state. *J. Crystal Growth*, 154, pp. 370-376 (October 1995).
- Selver, R., Kamotani, Y., and Ostrach, S., "Natural convection of a liquid metal in vertical circular cylinders heated locally from side." Accepted for presentation at ASME IMECE, 1996.
- Selver, R., Kamotani, Y., and Ostrach, S., "Natural convection of a liquid metal in vertical cylinders heated locally from side." Presented at the 1996 ASME International Congress and Exposition, Atlanta, 1996.
- Siegel, M. and Tanveer, S., Singular perturbation of smoothly evolving Hele-Shaw solutions. *Physical Review Letters*, (October 1996).
- Siegel, M. and Tanveer, S., Singular perturbation of smoothly evolving Hele-Shaw solutions. *Physical Review Letters*, (1996).
- Singhal, M., Bonetto, F., Lahey, R., "Phase distribution phenomena for simulated microgravity conditions: experimental work." NASA Contractor Report 198461, March 1996.
- Singhal, M., Bonetto, F., Lahey, R., Phase distribution phenomena for simulated microgravity conditions: experimental work. NASA Conference Publication, 3338, pp. 133-140 (1996).
- Skelton, A.C., McFadden, G.B., Impey, M.D., Riley, D.S., Cliffe, K.A., Wheeler, A.A., and Davis, S.H., On long-wave morphological instabilities in directional solidification. *Euro. J. Appl. Math.*, (1996).
- Slobozhanin, L., Alexander, J.I.D., and Resnick, A., "Stability of Liquid bridges under reduced gravity." Proceedings of the 2nd Symposium on Fluids in Space, Naples, Italy, April 22-26, 1996.
- Slobozhanin, L., Alexander, J.I.D. and Resnick, A., Bifurcation of the equilibrium states of a weightless liquid bridge. *Physics of Fluids*, (1996).
- Smedley, G.T., Wilemski, G., Rawlins, W.T., Oakes, D.B., Joshi, P., and Durgin, W.W., "Solute nucleation and growth in supercritical fluid mixtures." Third Microgravity Fluid Physics Conference, Cleveland, OH, June 13-15, 1996.
- Smith, M. and Glezer, A., "The development of novel, high-flux, heat transfer cells for thermal control in microgravity." Proceedings of Third Microgravity Fluid Physics Conference, Cleveland OH, June 13-15, 1996.
- Snyder, T.J., "Studies on the dielectrophoretic force and its effects on boiling bubble dynamics and heat transfer in terrestrial and microgravity environments." Washington State University, December 1995.
- Snyder, T.J. and Chung, J.N., Residual acceleration as a function of frequency for a 2.1 second drop tower with a "drag shield" design. *International J. of Microgravity Science & Technology*, vol. VIII, pp. 261-264 (December 1995).
- Snyder, T.J., Chung, J.N., and Schneider, J.B., "A study on the competing effects of the dielectrophoretic force and buoyancy on nucleate boiling heat transfer rates and on analogy with variable gravity boiling results." Proceedings of the ASME International Mechanical Engineering Conference, Atlanta, GA, November 17-22, 1996.
- Snyder, T.J., Schneider, J.B., and Chung, J.N., A second look at electrokinetic phenomena in boiling. *J. Applied Physics*, vol. 79, pp. 6755-6760 (1996).
- Solomentsev, Y., and Anderson, J.L. Electrophoretic Transport of Spheroidal Colloids in Nonhomogeneous Electric Fields. *I&EC Research*, vol. 34, 3231 (1995).
- Steen, Paul H., "Inviscid capillary breakup: collapse of the soap-film bridges." University of Dresden, Dresden, Germany, May 3, 1996.

- Steen, Paul H., "Inviscid capillary breakup: collapse of the soap-film bridges." ESPCI Paris, Paris, France, May 24, 1996.
- Steen, Paul H., "Inviscid capillary breakup: collapse of the soap-film bridge." University of Dresden, Dresden, GERMANY, 3 May 1996.
- Steen, Paul H., "Inviscid capillary breakup: collapse of the soap-film bridge." ESPCI Paris, Paris, FRANCE, May 24, 1996.
- Swinney, H.L., "Nonlinear dynamics seminar and physics department colloquium." Universidad Nacional Autonoma Mexico, Mexico City, August 13-14, 1996.
- Tanny, J., Chen, C.C., and Chen, C.F., Interaction between Marangoni and double - diffusive instabilities. *J. Fluid Mech.*, vol. 303, pp. 1-21 (1995).
- Tao, Y. and Kou, S., "Thermocapillary convection in low Pr materials under simulated reduced gravity." Third International Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, June 13-15, 1996.
- Tao, Y., Xiong, B., and Kou, S., Thermocapillary velocity in a molten NaNO_3 zone. (1996).
- Tennakoon, S. and Behringer, R.P. Onset of flow for horizontally shaken granular materials. *Phys. Rev. E.*, (submitted, 1996).
- Thiessen, D.B., Morse, S.F., Marr-Lyon, M.J., Marston, P.L., Capillary bridge modes driven with modulated acoustic radiation pressure. *Bulletin of the American Physical Society*, 40, 1923 (October 1995).
- Thompson, J.R., Drolet, F., and Vinals, J., "Fluid physics in a fluctuating acceleration environment." Proceedings of the Third Microgravity Fluid Physics Conference, Cleveland, OH, June 1996.
- Thomson, J.R. and Vinals, J., Statistical saturation of buoyant flow induced by a fluctuating acceleration. *AIAA J.*, vol. 34, pp. 975 (1996).
- Ting, C.-L. and Perlin, M., Boundary conditions in the vicinity of the contact line at a vertically oscillating upright plate: an experimental investigation. *Journal of Fluid Mechanics*, vol. 295, 263-300 (October 1995).
- Tong, P., "Polymer-induced depletion interaction and its effect on colloidal sedimentation in colloid-polymer mixtures." Proceedings of Third Microgravity Fluid Physics Conference 1996.
- Tong, P., "Polymer-induced depletion interaction and its effect on colloidal sedimentation in colloid-polymer mixtures." Third Microgravity Fluid Physics Conference, Cleveland, Ohio June 13-15, 1996.
- Tong, P., "Neutron scattering studies of interactions in mixtures of colloid and polymer." Physics Department Colloquium, University of North Texas, April 16, 1996.
- Tong, P., "Polymer-induced depletion interaction and its effect on colloidal sedimentation in colloid-polymer mixtures." Proceedings of Third Microgravity Fluid Physics Conference, NASA Conference Publication 3338, 413-418, July 13-15, 1996.
- Tong, P., "Polymer-induced depletion interaction and its effect on colloidal sedimentation in colloid-polymer mixtures." Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 13-15, 1996.
- Tong, P., "Velocity measurements in turbulent Thermal convection using lasers." Laser and Photonics Research Seminar, Laser Center, Oklahoma State University, August 8, 1996.
- Tong, P., "Interactions in mixtures of colloid and polymer." Workshop on Complex Fluids, China Center of Advanced Science and Technology, Beijing, China, September 23-28, 1996.
- Tong, P., Ye, X., and Huang, J. S., "Adsorption of end-functionalized polymer molecules on colloidal spheres." American Physical Society March Meeting, St. Louis, Missouri, March 18-22, 1996.

- Trau, M., Sankaran, D.A., and Aksay, I.A. Field-Induced Layering of Colloidal Crystals. *Science*, vol. 272, 706-709 (1996).
- Trau, M., Sankaran, S., Saville, D.A., and Aksay, I.A. Electric Field-Induced Pattern Formation In Colloidal Dispersions. *Nature*, vol. 374, 437-439 (1995).
- Trau, M., Sankaran, S., Saville, D.A., and Aksay, I.A. Pattern Formation in Non-Aqueous Colloidal Dispersions via Electrohydrodynamic Flow. *Langmuir*, 114665-114672 (1995).
- Tsao, H.-K. and Koch, D.L., Rapidly sheared, dilute gas-solid suspensions. *J. Fluid Mech.*, 296, pp. 211-245 (October 1995).
- Uphold, D.D., McKee, W. and McCready, M.J., "Examination of stability models for gas-liquid flow regime transitions." AIChE Annual Meeting, October 1995.
- Valiveti, P. and Koch, D.L., "Instabilities of bidisperse sedimenting gas-solid suspensions." American Physical Society Division of Fluid Dynamics Meeting, Syracuse, NY, 1996.
- VanHook, S.J., Schatz, M.F., McCormick, W.D., Swift, J.B., and Swinney, H.L., Long-wavelength instability in surface-tension-driven Benard convection. *Phys. Rev. Lett.*, 75, 4397-4400 (October 1995).
- VanHook, S.J., Schatz, M.F., McCormick, W.D., Swift, J.B. and Swinney, H.L., "Long-wavelength instability in Marangoni convection." Proceedings of the Third Microgravity Fluid Physics Conference, NASA LeRC, Cleveland, OH, 1996.
- VanHook, S.J., Schatz, M.F., McCormick, W.D., Swift, J.B., and Swinney, H.L. "Long-wavelength instability in Marangoni convection." Proceedings of the Proceedings of the Third Microgravity Fluid Physics Conference 1996.
- Velegol, D., and Anderson, J.L. Probing the Structure of Colloidal Doublets by Electrophoretic Rotation. *Langmuir*, vol. 12, 675 (1996).
- Velegol, D., and Anderson, J.L. Determining the Forces between Polystyrene Latex Spheres Using Differential Electrophoresis. *Langmuir*, vol. 12, 4103 (1996).
- Vera, M.U. and Durian, D.J., The angular distribution of diffusely transmitted light. *Phys. Rev. E* 53, 3215-3224 (1996).
- Vergeles, M., Keblinski, P., Koplik, J. and Banavar, J.R., Stokes drag and lubrication flows - a molecular dynamics study. *Phys. Rev. E* 53, 4852-4864 (1996).
- Vrane, D.R. and Smith, M.K. "The influence of domain curvature on the stability of viscously-dominated thermocapillary flows." *Advances in Multi-Fluid Flows*, Proceedings of the AMS-IMS-SIAM Joint Summer Research Conference on Multi-Fluid Flows and Interfacial Instabilities, 1996.
- Vrane, D.R. and Smith, M.K., "The influence of domain curvature on the stability of viscously-dominated thermocapillary flows." Forth-Eighth Meeting of the American Physical Society - Division of Fluid Dynamics, Irvine, CA, November 19-21, 1995.
- Wang, H. and Davis, R.H., Simultaneous sedimentation and coalescence of a dilute dispersion of small drops. *J. Fluid Mech*, 295, pp. 247-261 (October 1995).
- Wang, H. and Davis, R.H., Collective effects of gravitational and Brownian coalescence on droplet growth. *J. Colloid Interf. Sci*, 178, pp. 47-52 (1996).
- Wang, H. and Davis, R.H., Experiments on phase separation of dilute dispersions of coalescing drops. *J. Colloid Interf. Sci.*, 181, pp. 93-98 (1996).
- Wang, T.C., Snyder, T.J., and Chung, J.N., Experimental examination of forced-convection subcooled nucleate boiling and its application in microgravity. *ASME J. Heat Transfer*, vol. 118, pp. 237-241 (February 1996).

- Warren, J. A. and Murray, B. T., Ostwald ripening and coalescence of a binary alloy in two dimensions using a phase-field model. *Modelling Simul. Mater. Sci. Eng.*, 4, pp. 215-229 (1996).
- Weidner, Schwartz, L. and Eres, Simulation of coating layer evolution and drop formation on horizontal cylinders. *J. Colloid & Int. Sci.*, (1996).
- Weislogel, M., "Isothermal capillary phenomena." ZARM/Bremen University Colloquium Seminar Series, Bremen, Germany, November 1995.
- Weislogel, M., "Capillary flows: significance of the contact line boundary condition." ZARM/Bremen University Open Forum Seminar, Bremen, Germany, November 1995.
- Weislogel, M.M., Capillary flow in an interior corner, UMI dissertation information service. Ph.D thesis, Northwestern University, Evanston, IL, (1996).
- Weislogel, M.M., Capillary flow in an interior corner, UMI dissertation information service. Ph.D thesis, Northwestern University, Evanston, IL. NASA Tech Brief, (1996).
- Wettlaufer, J.S., Worster, M.G., Wilen, L.A., and Dash, J.G., A theory of premelting dynamics for all power law forces. *Phys Rev. Lett.* 76, 3602, (1996).
- Wheeler, A.A., McFadden, G.B., and Boettinger, W.J., Phase-field model for solidification of a eutectic alloy. *Proc. R. Soc. Lond. A*, 452, pp. 495-525 (1996).
- Witte, L.C., "Fluid dynamics and heat transfer in falling films." Texas A&M University, October 9, 1995.
- Witte, L.C., Bousman, W.C., and Fore, L.B., "Studies of two-phase flow dynamics and heat transfer at reduced gravity conditions." NASA Contractor Report 198459, February 1996.
- Wright, W.B., Budakian, R., and Putterman, S., "Resolving high amplitude surface motion with diffusing light." *Proceedings of the 3rd Microgravity Fluids Conference Proceedings*, NASA Lewis Research Center, R. Ziegfeld ed., June 13-15, 1996.
- Wright, W.B., Budakian, R., and Putterman, S.J., Diffusing light photography of fully developed isotropic ripple turbulence. *Physical Review Letters*, vol. 76, 4528- 4531 (June 10, 1996).
- Wu, X-l., Martin, B., and Tharrington, A. Second Microgravity Fluid Physics Conference Proceedings, NASA Conference Publication 3276, p 319.
- Wu, X-l., Martin, B., Kellay, H., and Goldburg, W.I. Hydrodynamic Convection in a Two-dimensional Couette Cell. *Phys. Rev. Lett.*, vol. 75, 236 (1995).
- Xu, J. and Zebib, A., "Stability analysis of thermocapillary convection in rectangular cavity ." ASME-IMECE, Atlanta, GA, November, 1996.
- Xu, J. and Zebib, A., "Nonlinear stability of thermocapillary convection in a rectangular cavity." 48th Annual Meeting of the APS/DFD, Irvine, CA, November 19-21, 1995.
- Y. Tao, B. Xiong and S. Kou, Thermocapillary velocity field in a silicone oil zone. *International Journal of Heat and Mass Transfer*, (1996).
- Ye, X., Narayanan T., Tong, P., and Huang, J.S., Neutron scattering study of depletion interactions in a colloid-polymer mixture. *Phys. Rev. Lett.*, 76, 4640 (1996).
- Ye, X., Narayanan, T., Tong, P., Huang, J. S., Lin M. Y., Carvalho, B. L., and Fetters, L. J., Depletion interaction in colloid-polymer mixtures. *Phys. Rev. E.*, (accepted, 1996).
- Zebib, A., "Thermocapillary instabilities with system rotation." 49th Annual Meeting of the APS/DFD, Syracuse, NY, November 24-26, 1996.

Zhang, N. and Chai, A.T., "Effects of evaporation on thermocapillary flows in liquid thin layer." 4th International Symposium on Heat Transfer, Beijing, China, October 4 - 11, 1996.

Zhang, N. and Chai, A.T., "Marangoni-Benard convection in an evaporating liquid thin layer." 4th International Symposium on Heat Transfer, October 4 - 11, 1996, Beijing, China.

Zhang, N. and Chai, A.-T. "Effects of Evaporation on Thermocapillary Flows in a Liquid Thin Layer," in "Heat Transfer Science and Technology." Edited by: Wang Buxuan Higher Education Press, Beijing, China, pp 329-334, 1996.

Zhang, W. and Vinals, J., Square patterns and quasi-patterns in Faraday waves in low viscosity fluids. *Phys. Rev. E*, vol. 53, R4283, (1996).

Zhang, W. and Vinals, J., Pattern formation in weakly damped Faraday waves. *J. Fluid Mech.* (in press).

Zhao, H., Sadhal, S.S., and Trinh, E.H. "Singular perturbation analysis of an acoustically levitated sphere." Western States Section of the Combustion Institute, Fall 1996 Meeting, Los Angeles, October 1996, Paper No. 96F-126.

Zhou, H. and Davis, R.H., Axisymmetric thermocapillary migration of two deformable viscous drops. *J. Colloid Interf. Sci.*, 181, pp. 60-72 (1996).

Zhou, L.-M., On stability of a catenoidal liquid bridge. *Pacific J. Math.*, (in press, 1996).

Zielinski, R.G., Paulaitis, M.E., and Kaler, E.W., Isopycnic phases in supercritical fluid / water / C₁₂E₁₀ mixtures. *J. Phys. Chem.*, 100, 9465 (1996).

Zielinski, R.G., Paulaitis, M.E. and Kaler, E.W., A new cell for neutron scattering at elevated pressures. *Rev. Sci. Instr.*, 67, 2612 (1996).

Zinchenko, A.Z., and Davis, R.H., Collision efficiency of drops and solid spheres in a shear flow at arbitrary Peclet numbers. *Phys. Fluids*, 7, pp. 2310-2327 (October 1995).

Zinchenko, A.Z., Rother, M.A., and Davis, R.H., "Coalescence rate of slightly deformable drops in a gravitational field." AIChE Meeting, Miami, FL, November 1996.

Ground: Fundamental Physics

Ahlers, G. and Liu, F.-C. "4He very near T_l heated from above." Proceedings of the 21st International Conference on Low Temperature Physics LT-21 (Prague), Czechoslovak Journal of Physics, vol. 46-Suppl, 187 (1996).

Baddar, H., Fu, H., Larson, M., Mulders, N., and Ahlers, G. "A High-Resolution Susceptibility Thermometer for use Near 2 K." Proceedings of the 21st International Conference on Low Temperature Physics LT-21 (Prague), Czechoslovak Journal of Physics, vol. 46-Suppl, 2859 (1996).

Baddar, H., Fu, H., Liu, F.-C., and Ahlers, G. "The Thermal Boundary Resistance in Superfluid 4He Near T_l." Proceedings of the 21st International Conference on Low Temperature Physics LT-21 (Prague), Czechoslovak Journal of Physics, vol. 46-Suppl, 191 (1996).

Baddar, H., Fu, H., Liu, F.-C., and Ahlers, G. "The Thermal Boundary Resistance of 4He near T_l." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop, NASA Document D-13845.

Bouyer, P., Gustavson, T., Haritos, K., and Kasevich, M. Microwave signal generation with optical injection locking. *Optics Letters*, vol. 21, 1502 (1996).

Bouyer, P., Gustavson, T., Haritos, K., and Kasevich, M. Sensing inertial forces with laser manipulated atoms. *IEEE/LEOS Newsletter*, vol. 9, 22 (1995).

Bouyer, P., Gustavson, T., Haritos, K. G., McGuirk, J., Thompson, M., and Kasevich, M. "Atom interferometer-based navigation systems." Proceedings of the International Symposium for Optronics and Defense (1996).

- Bouyer, P., Gustavson, T., Haritos, K., McGuirk, J., and Kasevich, M. "Atom interferometry in a microgravity environment." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13845, 146 (1996).
- Chui, Talso C. P., Goodstein, David L., Harter, Alexa W., and Mukhopadhyay, Ranjan "Heat Capacity of Superfluid 4He in the Presence of a Heat Current near Tl." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13485 (1996).
- Cowan, M., Rudnick, J., and Barmatz, M. Effects of random motions on critical point measurements: liquid-gas systems in microgravity. *Physical Review E*, vol. 53, 4490 (1996).
- Donnelly, R. J. "The Field of Low Temperature Physics." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13485 (1996).
- Donnelly, R. J. "Low Temperature Physics." The London Lectures, Duke University, March 1996.
- Ferrell, R. A. "A brief survey of the equilibrium and transport properties of critical fluids and the degree to which microgravity is required for their experimental investigation." Proceedings of the Third Microgravity Fluid Physics Conference, Cleveland, June 1996, NASA conference publication 3338, 53-57 (1996).
- Ferrell, R. A. "Modulated order parameter." Max Planck Institut fuer Physik Komplexer Systeme, Dresden, Germany, June 1996.
- Frank, D.J. "Dynamics of superfluid helium in low gravity: A progress report." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA Document D-13845 (1996).
- Fu, H., Baddar, H., Larson, M., Mulders, N., and Ahlers, G. "A high-resolution thermometer using a DC SQUID." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop, NASA Document D-13845.
- Goodstein, David, Chui, Talso C. P., and Harter, Alexa Heat flow induced anomalies in superfluid 4He near Tl. *Physical Review Letters*, 77, 979 (1996).
- Hahn, I., Gonzalez, A., and Barmatz, M. "Fuzzy logic controller for low temperature applications." Proceedings of the 21st International Low Temperature Physics Conference LT-21 (Prague), Czechoslovak Journal of Physics vol. 46 (1996).
- Halley, J. W. "Progress and Prospects for the 4He Condensate Experiment." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop, NASA Document D-13845 (1996).
- Halley, J. W. "Prospects for an Ultralow Pressure Gauge Based on Brownian Motion of a Suspended Particle." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop, NASA Document D-13845 (1996).
- Halley, J. W. "Computational and Experimental Explorations of the Possibility of Condensate Mediated Absorption and Reemission in Superfluid Helium Four." Workshop on Quantum Evaporation, Pisa, Italy, December 13-17, 1995.
- Halley, J. W. "Progress and Prospects for the 4He Condensate Experiment." 1996 NASA/JPL Low Temperature Microgravity Workshop, Pasadena, April 9-11, 1996.
- Halley, J.W. "Prospects for an Ultralow Pressure Gauge Based on Brownian Motion of a Suspended Particle." 1996 NASA/JPL Low Temperature Microgravity Workshop, Pasadena, April 9-11, 1996.
- Heinzen, D. "Ultra-precise measurements with nanokelvin atoms in a microgravity environment." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13845 (1996).
- Johnson, T. A., and Elbaum, C. Nucleation of a non-equilibrium phase in a first order phase transition. *Journal of Low temperature Physics*, in press, (1996).
- Johnson, T.A. and Elbaum, C. "Nucleation of a non-equilibrium phase in a first-order phase transition: Bcc ⁴He from superfluid." American Physical Society March Meeting, St. Louis, MO, March 18-22, 1996.

- Kasevich, M. "Precision measurements with atom interferometers." Physics Colloquium, Los Alamos National Laboratory, July 1996.
- Kasevich, M. "Rotation measurements with atom interferometer gyroscopes." Workshop on Atom Optics and Interferometry, Cairns, Australia, July 1996.
- Kasevich, M. "Precision measurements of inertial forces using atom interferometry." Atomic Physics Seminar, University of Texas, Austin, April 1996.
- Kasevich, M. "Measuring inertial forces with precision atom interferometry." Institute of Theoretical Physics Colloquium, Santa Barbara, March 1996.
- Kasevich, M. "Using atom interferometers to measure inertial forces: gyroscopes and accelerometers." Atomic Physics Seminar, University of Oregon, Eugene, March 1996.
- Kogan, A.B., Zhong, F. and Meyer, H. "Dynamics of density equilibration near the liquid-vapor critical point of ^3He ." Proceedings of the 21st International Conference on Low Temperature Physics LT-21 (Prague), Czechoslovak Journal of Physics, vol. 46, Supplement S1 (1996).
- Larson, M., Liu, F.-C., and Israelsson, U. E. "Reducing gravity at the superfluid transition in ^4He ." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13845, 64-65 (1996).
- Liu, F.-C. , and Ahlers, G. A new dissipative region below the superfluid transition of ^4He in a heat current. Physical Review Letters, vol. 76, 1300 (1996).
- Liu, F.-C., and Ahlers, G. "Thermal Resistance below the Superfluid Transition of ^4He in a Heat Current." Proceedings of the 21st International Conference on Low Temperature Physics LT-21, Czechoslovak Journal of Physics, vol. 46-Suppl, 189 (1996).
- Liu, F.-C., and Ahlers, G. " ^4He very near TI heated from above." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop, NASA Document D-13845.
- Manousakis, E., and Schultke, N. "Scaling in confined helium: geometry and boundary effects." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13845, 23-27 (1996).
- Maris, H. J., Weilert, M. A., Whitaker, D. L., and Seidel, G. M. "Magnetic levitation of liquid helium." Proceedings of the 21st International Conference on Low Temperature Physics LT-21 (Prague), Czechoslovak Journal of Physics, vol. 46, Supplement S1, 373 (1996).
- Mulders, N., Larson, M., and Nash, A. "Experiments near the tricritical point in ^3He - ^4He mixtures." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop, NASA Document D-13845, 83-84 (1996).
- Schultka, N., and Manousakis, E. "Boundary effects on the scaling of the superfluid density." Proceedings of the 21st International Conference on Low Temperature Physics LT-21, Czechoslovak Journal of Physics, vol. 46 - Supplement S1, 451 (1996).
- Schultka, N., and Manousakis, E. Specific heat of superfluids near the transition temperature. Physical Review B, vol. 52, 7528 (1996).
- Schultka, N., and Manousakis, E. Scaling of the specific heat of superfluid films. Physical Review Letters, vol. 75, 2710 (1995).
- Schultka, N., and Manousakis, E. Three-dimensional X-Y model with a Chern-Simons term. Physical Review B, vol. 53, 4782 (1996).
- Strayer, D. M., Jiang, W., Yeh, N.-C., and Asplund, N. N. "Precision density measurements near the helium lambda transition using high-Q microwave cavities." 1996 March Meeting of the American Physical Society, St. Louis, March 20-24, 1996.

- Weilert, M. A., Whitaker, D. L., Maris, H. J., and Seidel, G. M. "Magnetic levitation and non-coalescence of helium drops." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop, NASA document, D-13845, 193-195 (1996).
- Williams, M. C., Giese C. F. and Halley, J. W. Suspension of Superfluid Helium Using Cesium-Coated Surfaces. Physical Review B, vol. 53, 6627 (1996).
- Yeh, N.-C., Jiang, W., Strayer, D. M., and Asplund, N. N. "Precise measurements of the density and critical phenomena near the phase transitions in helium using high-Q niobium microwave cavities." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Physics Workshop, NASA document D-13845, 98-99 (1996).
- Yeh, N.-C., Jiang, W., Strayer, D. M., and Asplund, N. N. "Precise measurements of the density and critical phenomena near the phase transitions in helium using high-Q niobium microwave cavities." Proceedings of the 21st International Low temperature Physics Conference LT-21 (Prague), Czechoslovak Journal of Physics, vol. 46, Supplement S1, 181-2
- Young, B., Kasevich, M., and Chu, S. "Atom Interferometry." Edited by: Berman, P., Chapter: Precision measurement with light pulse atom interferometers.
- Zhong, F., and Meyer, H. Density equilibration near the liquid-vapor critical point of a pure fluid. II. Coexisting phases for $T < T_c$. Physical Review E, 53, 5935 (1996).
- Zhong, F. and Meyer, H. "Density equilibration near the liquid-vapor critical point of ^3He II: Coexisting phases $T < T_c$." Proceedings of the 1996 NASA/JPL Low Temperature Microgravity Workshop.

Ground: Materials Science

- Ainsworth, P.J. and Gupta, P.K. "Influence of free convection in dissolution." Annual meeting of the American Ceramics Society, Indianapolis, IN 1996, Ceramic Bulletin, 75, p267.
- Aldrich, D.J., and Reagey, D.W., "Vapor phase sintering in multicomponent systems." American Ceramic Society Annual Meeting, Indianapolis, IN, May 1996.
- Aldrich, D.J., and Readey, D.W., "Vapor phase sintering of multicomponent ceramics." Poster Presentation at Rocky Mountain Chapter Meeting of the American Vacuum Society, 1st Place Prize in Student Division, 1996.
- Aldrich, D.J., Ritland, M. A., and Readey, D.W., "Vapor phase sintering of ceramics." Ceramographic Exhibit, American Ceramic Society Annual Meeting, Indianapolis, IN, 2nd place. SEM category, May 1996.
- Alexander, J.I.D., "Response of crystal growth experiments to time-dependent residual acceleration." Proceedings of the 9th European Symposium on Gravity Dependent Phenomena in Physical Sciences, vol. 464, eds. L. Ratke, H. Walter and B. Feuerbacher (Springer Verlag, Berlin) 95-105, 1996.
- Alexander, J.I.D., Scaling and estimation of experiment response to g-jitter. Microgravity Quarterly, vol. 5, (November 1, 1995).
- Alexander, J.I.D., "Quantitative experimental characterization of g-jitter effects on directional solidification." presented at the 31st Annual COSPAR meeting, Birmingham, England, July 14-21, 1996.
- Alexandrou, A., Gatsonis, N., Durgin, W., and Sacco, Jr., A. "Modeling of Macroscopic/Microscopic Transport Phenomena In Zeolite Crystal Solutions Under Microgravity Conditions." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.
- Allen, D.R., and Perepezko, J.H. "Kinetic Competition During Duplex Partitionless Solidification." ASM/TMS Fall Meeting, Cincinnati, October 1996.
- Allen, D.R., and Perepezko, J.H. "Kinetic Competition During Duplex Partitionless Solidification (invited seminar)." Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland, August 1996.

- Allen, D.R. and Perepezko, J.H. "Kinetic competition during duplex partitionless solidification in Ni-V alloys." *Thermodynamics and Kinetics of Phase Transformations* 398, Proceedings of the Materials Research Society Symposium, J.S. Im, B. Park, A.L. Greer, and G.B. Stephenson eds., 57 (1996).
- Allen, D.R. and Perepezko, J.H. "Kinetic competition during duplex partitionless solidification." *ASM/TMS Fall Meeting*, Cincinnati, OH, October, 1996.
- Allen, D.R. and Perepezko, J.H. "Kinetic competition during duplex partitionless solidification." *Ecole Polytechnique Federale de Lausanne*, Lausanne, Switzerland, August 1996.
- Allen, D.R. and Perepezko, J.H. "Kinetic competition during duplex partitionless solidification in Ni-V alloys." *Materials Research Society Fall Meeting*, Boston, MA, November, 1995.
- Allen, D.R., Gremaud, M., and Perepezko, J.H. "Nucleation Controlled Microstructural Development in Al-Si Alloys." *Ninth International Conference on Rapidly Quenched and Metastable Materials*, Bratislava, Slovakia, August 1996.
- Allen, D.R., Gremaud, M. and Perepezko, J.H. "Nucleation controlled microstructural development in Al-Si alloys." *Ninth International Conference on Rapidly Quenched and Metastable Materials*, Bratislava, Slovakia, August 1996.
- Anderson, T.J., and Narayanan, R. "A Novel Electrochemical Method for Flow Visualization." *Microgravity Materials Science Conference*, Huntsville, Alabama, June 10-11, 1996.
- Andrews, B., and Coriell, S. "The Effect of Convection on Morphological Stability During Coupled Growth in Immiscible Systems." *Microgravity Materials Science Conference*, Huntsville, Alabama, June 1996.
- Andrews, B., and Coriell, S. "The Effect of Convection on Morphological Stability During Coupled Growth in Immiscible Systems." *Extended Abstract, Microgravity Materials Science Conference, Report Summaries Volume*, 32-33, 1996.
- Apfel, R., and Qui, N. *Principle of dynamic decompression and cooling for materials processing*. vol. 11, (1996).
- Arnold, S., Holler, S., Li, J.H., Serpengzel, A., Auffermann, W.F., and Hill, S.C. *Aerosol Particle Microphotography and Glare Spot Absorption Spectroscopy*. *Opt. Lett.*, 20, 773-775 (1995).
- Arnold, S., Li, J.H., Holler, S., Korn, A., and Izmailov, A.F. *Recording Long-Term Optical Images of a Brownian Particle in a Paul Trap essentially free of Thermally Induced Positional Noise*. *J. Appl. Phys.*, 76, 1 (1995).
- Avci, D., and Mathias, L.J. *Cyclopolymerization of Cinnamate Ester Derivates of Alkyl α -(Hydroxymethyl) Acrylates*. *Polymer Bulletin*, vol. 35, 671 (1995).
- Avci, D., and Mathias, L.J. *Examples of New Synthetic Routes to Pendant Ester-Ether Derivatives of α -Hydroxymethylacrylate Polymers*. *Polymer Bulletin*, vol. 3, no. 2, 133 (1996).
- Avci, D., Thigpen, K.T., and Mathias, L.J. *Effects of Reduced Gravity on the Molecular Weight of Photopolymerized Methyl Methacrylate*. *Polymer Preprints*, vol. 37, no. 2, 317 (1996).
- Avci, D., Thigpen, K.T., and Mathias, L.J. "Effects of Reduced Gravity on the Molecular Weight of Photopolymerized Methyl Methacrylate." *ACS National Meeting*, Orlando, Florida, August 25-29, 1996.
- Avci, D., Thigpen, K.T., and Mathias, L.J. *Photopolymerization Studies of Alkyl and Aryl Ester Derivatives of Ethyl α -Hydroxymethylacrylates*. *J. Poly. Sci., Polym. Chem. Ed.*, vol. 34, no. 5, 3191 (1996).
- Aziz, M.J. "Pressure- and stressed-enhanced kinetics." *International Conference on Diffusion in Materials*, Nordkirchen, Germany, August 1996.
- Aziz, M.J. "Rapid solidification." *Advanced Technology Research Laboratories*, Nippon Steel, Kawasaki, Japan, March 1996.
- Aziz, M.J. "Rapid solidification." *Central Research Laboratories*, Kobe Steel, Kobe, Japan, March 1996.

- Aziz, M.J. "Rapid solidification." Central Research Laboratories, Matsushita Electric Industrial Company, Kyoto, Japan, March 1996.
- Aziz, M.J. "Research opportunities in highly nonequilibrium growth by pulsed laser deposition." Institute of Materials Science, University of Tsukuba, Tsukuba, Japan, March 1996.
- Aziz, M.J. "Fundamental issues in nonequilibrium growth by pulsed laser deposition." Research Laboratory of Engineering Materials, Tokyo Institute of Technology, Yokohama, Japan, March 1996.
- Aziz, M.J. "Experimental constraints on nonequilibrium interface kinetic models." Ninth International Conference on Rapidly Quenched and Metastable Materials, Bratislava, Slovakia, August 1996.
- Aziz, M.J. "Pressure- and stressed-enhanced kinetics. International Conference on Diffusion in Materials." Nordkirchen, Germany, August 1996.
- Aziz, M.J. "Rapid solidification." Advanced Technology Research Laboratories, Nippon Steel, Kawasaki, Japan, March 1996.
- Aziz, M.J. "Rapid solidification." Central Research Laboratories, Kobe Steel, Kobe, Japan, March 1996.
- Aziz, M.J. "Rapid solidification." Central Research Laboratories, Matsushita Electric Industrial Company, Kyoto, Japan, March 1996.
- Aziz, M.J. "Research opportunities in highly nonequilibrium growth by pulsed laser deposition." Institute of Materials Science, University of Tsukuba, Tsukuba, Japan, March 1996.
- Aziz, M.J. "Research opportunities in highly nonequilibrium growth by pulsed laser deposition." Institute of Materials Science, University of Tsukuba, Tsukuba, Japan, March 1996.
- Aziz, M.J. "Fundamental issues in nonequilibrium growth by pulsed laser deposition." Research Laboratory of Engineering Materials, Tokyo Institute of Technology, Yokohama, Japan, March 1996.
- Aziz, M.J. "Experimental constraints on nonequilibrium interface kinetic models." Ninth International Conference on Rapidly Quenched and Metastable Materials, Bratislava, Slovakia, August 1996.
- Balwada, H., and McGinn, P. " Y_2BaCuO_5 Particle Segregation in Zone Melt Textured $\text{YBa}_2\text{Cu}_3\text{O}_{7.8}$." MISCON Group Meeting, Univ. of Notre Dame, Notre Dame, Indiana, August 1996.
- Bassler, B.T., Hofmeister, W.H., and Bayuzick, R.J. "Examination of Solidification Velocity Determination in Bulk Undercooled Nickel." MRS Fall Meeting, Boston, Massachusetts, December 1995.
- Beatty, K.M., and Jackson, K.A. "Orientation Dependence of the Distribution Coefficient (k-value) Obtained from a Spin-1 Ising Model." Tenth American Conference on Crystal Growth, Vail, Colorado, August 6, 1996.
- Beckermann, C. and Wang, C.Y., "Modeling of microstructure formation in alloy solidification with convection." JIM Annual Meeting, 1996.
- Becla, P., Witt, A.F., Lagowski, J., and Walukiewicz, W. Large photo-induced persistent optical absorption in Se doped AlSb. *Appl. Phys. Lett.*, 67, (3), 395-397 (1995).
- Biswas, A.B., Weber, J.K.R., and Nordine, P.C. Cr^{3+} Fluorescence in Containerless Melt-purified Aluminum Oxide. *J. Mat. Res.*, vol. 10, 1823-1827 (1995).
- Blackmore, K., Beatty, K.M., Hui, M., and Jackson, K.A. "Growth Behavior of $\text{NH}_4\text{Cl-H}_2\text{O}$ Mixtures." Tenth American Conference on Crystal Growth, Vail, Colorado, August 8, 1996.
- Boatner, L.A., Corrigan, D., David, S.A., Rappaz, M., Workman, G., and Smith, G. "Surface Morphological Properties of Stationary Melt Pools in Single Crystals of Stainless Steel." NASA Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.

- Brady, J.F. "Dispersion Microstructure and Rheology in Ceramics Processing (poster exhibit)." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.
- Brezinsky, K. "Gas-Phase Combustion Synthesis of Materials." Twenty-Sixth Symp. (Int.) Comb., The Combustion Institute (1996).
- Brezinsky, K., Brehm, J.A., Law, C.K., and Glassman, I. "Supercritical Combustion Synthesis of Titanium Nitride." Twenty-Sixth Symp. (Int.) Comb., The Combustion Institute (1996).
- Brezinsky, K., Brehm, J.A., Law, C.K., and Glassman, I. "Supercritical Combustion Synthesis of Titanium Nitride." 1996 Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.
- Ceccio, S. L., Tryggvason, G., Han, J., Che, J., and Juric, D., "Fundamentals of mold free casting: experimental and numerical studies." poster presentation at the Microgravity Materials Science Conference, Huntsville, Alabama, 1996.
- Cezairliyan, A. "Thermophysical Properties of High Temperature Liquid Metals and Alloys." NASA Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.
- Cezairliyan, A., and Righini, F. Issues in High-Speed Pyrometry. *Metrologia*, vol. 33, 299-306 (1996).
- Chang, S., and Stefanescu, D.M. A model for inverse segregation: The case of directionally solidified Al-Cu alloys. *Acta mater.*, vol. 44, no. 6, 2227-2235 (1996).
- Chang, S., and Stefanescu, D.M. A model for macrosegregation and its application to Al-Cu castings. *Metallurgical and Materials Transactions*, vol. 27A, 2708-2721 (1996).
- Che, J., Han, J., Tryggvason, G., and Ceccio, S.L., "Liquid metal drop impingement." presented at the American Physical Society Division of Fluid Dynamics Meeting, Syracuse, New York, 1996.
- Chen, M.T. and Dahm, A.J., Optical cell for observing solidification of helium. *Cryogenics*, 35, 71, (October 1995).
- Chung, H., Raghothamachar, B., Dudley, M., and Larson, Jr., D.J. "Synchrotron White Beam X-Ray Topography Characterization of Structural Defects in Microgravity and Ground Based CdZnTe crystals (in "Space Processing of Materials")." *SPIE Proceedings*, vol. 2809, 45-56 (1996).
- Chung, H., Raghothamachar, B., Wu, J., Dudley, M., Larson, Jr., D.J., and Gillies, D.C. "Characterization of Growth Defects in CdZnTe Single Crystals by Synchrotron White Beam X-ray Topography, in "Defect and Impurity-Engineered Semiconductors and Devices" (S. Ahok, J. Chevallier, I. Akasaki, N.M. Johnson, and B.L. Sopori, Eds.)." *Mat. Res. Soc.*
- Chung, H., Raghothamachar, B., Zhou, W., Dudley, M., and Gillies, D.C. "Studies of Interface Demarcation and Structural Defects in Ga doped Ge Single Crystals by Synchrotron White Beam X-Ray Topography (in "Applications of Synchrotron Radiation to Materials Science," L. Terminello, S. Mini, D. L. Perry, and H. Ade, eds.)." *Mat. Res. Soc. Symp. Proc.*, 437
- Clark, I.O., Hyer, P.V., and Johnson, E.J. "Thermal imaging for enhanced semiconductor process yield." *Technology 2006*, Anaheim, CA, October 29-31, 1996.
- Clark, I.O., Jesser, W.A., Hyer, P.V. and Johnson, E.J. "Microgravity chemical vapor deposition." Microgravity Materials Science Conference, Huntsville, AL, June 10-11, 1996.
- Cook, K.D., Festag, R., Wunderlich, B., Joy, D.C., and Alexandratos, S.D. "Separation and characterization of single-chain polymer particles." *SPIE Annual Meeting*, Denver, Colorado, August 4-8, 1996.
- Cooper, R.F. "Dynamic redox reactions and the formation of fine-grained, polycrystalline oxide/silicate ceramics from inviscid melts." In: *Space Processing of Materials*, edited by N. Ramachandran. *Proc. SPIE*. 2809:69-77 (1996).
- Cooper, R.F., Fanselow, J.B. and Poker, D.B. The mechanism of oxidation of a basaltic glass: Chemical diffusion of network-modifying cations. *Geochim Cosmochim. Acta*, 60, 3253-3265 (1996).

Cooper, R.F., Fanselow, J. B., Weber, J.K.R., Merkley, D.R. and Poker, D.B. Dynamics of oxidation of a Fe-bearing aluminosilicate (basaltic) melt. *Science*, 274 (1996).

Covert, H. and Brown, R.A. Dynamics of small-scale floating zones: The thermal capillary limit. MIT Report, (1996).

Curreri, P.A., and Kaukler, W. Real-Time X-Ray Transmission Microscopy of Solidifying Al-In Alloys. *Metallurgical Transactions*, vol. 27A, no. 3, 801-808 (1996).

Curreri, P.A., and Kaukler, W. "X-Ray Transmission Microscopy Study of the Dynamics of Solid/Liquid Interfacial Breakdown During Metal Alloy Solidification." *Proceedings of the 8th International Symposium on Experimental Methods for Microgravity Materials Science*, 125 TMS Annual Meeting, Anaheim, California, February 4-8, 1996.

Dold, P., Cröll, A., Szofran, F., Kaiser, Th., and Benz, K.W. "Growth of semiconductor crystals: comparison between the effect of microgravity and magnetic fields." *Proceedings of the Third China-Japan Workshop on Microgravity Science*, Xian, China, October, 1996.

Dold, P., Cröll, A., Szofran, F., Kaiser, Th., and Benz, K.W. "Growth of semiconductor crystals: comparison between the effect of microgravity and magnetic fields." Presented at the Third China-Japan Workshop on Microgravity Science, Xian, China, October, 1996.

Dudley, M., Larson Jr., D.J., Chung, H., and Raghothamachar, B. "Characterization of Zn-Alloyed CdTe Compound Semiconductors Processed in Microgravity on USML-1 and USML-2." *Proceedings of 31st COSPAR Scientific Assembly*, Birmingham, United Kingdom, July 14-21, 1996 ("Advances in Space Research").

Dulikravich, G.S. "An unified theory of electro-magneto-gas dynamics." *Hypersonics MAGLEV Group Meeting*, National High Magnetic Field Laboratory, Tallahassee, Florida, December 1995.

Dulikravich, G.S., and Lynn, S.R. "Electro-Magneto-Hydrodynamics: Part 1 - Introductory Concepts." *Symposium on Developments in Electro-Rheological Flows-1995*, D.A. Siginer and G.S. Dulikravich, eds., ASME WAM '95, San Francisco, California, November 12-17, 1995, ASME FED-Vol. 235, MD-Vol. 71, pp 49-58.

Dulikravich, G.S., and Lynn, S.R. "Electro-Magneto-Hydrodynamics: Part 2 - A Survey of Mathematical Models." *Symposium on Developments in Electro-Rheological Flows-1995*, D.A. Siginer and G.S. Dulikravich, eds., ASME WAM '95, San Francisco, California, November 12-17, 1995, ASME FED-Vol. 235, MD-Vol. 71, pp 59-70.

Duval, W.M.B., "Flow field topology of buoyancy induced mixing." *AIAA-96-0253*, 34th Aerospace Sciences Meeting & Exhibit, Reno, NV., January 15-18, 1996.

El-Shall, M.S. "Studies on nucleation, polymerization, and nanoparticle composites in supersaturated vapors under microgravity." *NASA Microgravity Materials Science Conference*, Huntsville, Alabama, June 10-12, 1996.

El-Shall, M.S. "From clusters to polymers and nanoparticles: a route to novel materials." *70th American Chemical Society Colloid and Surface Science Symposium*, Clarkson University, Potsdam, New York, June 16-19, 1996.

El-Shall, M.S. "Surface oxidation and luminescence properties of weblike agglomeration of silicon nanocrystals produced by a laser vaporization - controlled condensation technique." *Fifth Annual Meeting of the Consortium for Nanostructured Materials*, Vanderbilt University, Nashville, Tennessee, October 18-19, 1996.

Festag, R., Alexandratos, S.D., Cook, K.D., Joy, D.C., Phillips, P.J., and Wunderlich, B. "Synthesis and characterization of single macromolecules: Mechanistic studies of crystallization and aggregation." *Microgravity Materials Science Conference*, Report Summaries Volume, 24-25 (1996).

Festag, R., Alexandratos, S.D., Cook, K.D., Joy, D.C., Phillips, P.J., and Wunderlich, B. "Synthesis and characterization of single macromolecules: Mechanistic studies of crystallization and aggregation." *Microgravity Materials Science Conference*, Huntsville, Alabama, June 10-11, 1996.

Festag, R., Wunderlich, B., Alexandratos, S.D., and Cook, K.D. "Separation and Characterization of Single-Chain Polymer Particles." *American Physical Society, March Meeting*, St. Louis, Missouri, March 18-22, 1996.

Festag, R., Wunderlich, B., Joy, D.C., Alexandratos, S.D., and Cook, K.D. "Separation and characterization of single-chain polymer particles (in "Space Processing of Materials," N. Ramachandran, ed.)." *Proceedings of SPIE* 2809, 155-165 (1996).

Frazier, D.O., Hung, R.J., Paley, M.S., and Long, Y.T. Effects of Convection During the Photodeposition of Polydiacetylene Thin Films. *J. Crystal Growth*, (1996, accepted).

Garandet, J.P., Corre, S., Gavaille, S., Favier, J.J., and Alexander, J.I.D., On the effect of gravity perturbations on composition profiles during Bridgman crystal growth in space. *J. Crystal Growth*, (1996).

Grasza, K., Trivedi, S.B., Yu, Z., Kutcher, S.W., Palosz, W., and Brost, G.A. "Low supersaturation nucleation and 'contactless growth of photorefractive ZnTe crystals." *ACCG-10/ICVGE-9*, Vail, Colorado, August 1996.

Gremaud, M., Allen, D.R., M. Rappaz, M., and Perepezko, J.H. The development of nucleation controlled microstructures during laser treatment of Al-Si alloys. *Acta Materialia*, 44, 2669 (1996).

Grugel, R.N. "Novel Directional Solidification Processing of Hypermonotectic Alloys (poster presentation)." *Microgravity Materials Science Conference*, Huntsville, Alabama, June 10-11, 1996.

Grugel, R.N. "Utilizing Controlled Vibrations in a Microgravity Environment to Understand and Promote Microstructural Homogeneity During Floating-zone Crystal Growth (poster presentation)." *Microgravity Materials Science Conference*, Huntsville, Alabama, June 10-11, 1996.

Guzman, J.A., Moore, J.J., and Readey, D.W., "Effects of liquid metals during combustion synthesis in the Ti-Ta-B system." *American Ceramic Society, Annual Meeting*, Indianapolis, April 14-17, 1996.

Haas, C.K., and Torkelson, J.M. 2D vs. 3D coarsening in phase-separated polymer solutions: Dependence on distance from criticality and interfacial tension. *ACS Polymer Preprints*, vol. 36, no. 2, 360 (1995).

Haas, C.K., and Torkelson, J.M. 2D coarsening in phase-separated polymer solutions: Dependence on distance from criticality. *Phys. Rev. Lett.*, vol. 75, 3134 (1995).

Han, J., Tryggvason, G., and Ceccio, S.L., The heat loss of a drop colliding with a cold wall. *ASME J. Heat Transfer*, (1996).

Hansen, G., Hellawell, A., Lu, S.Z., and Steube, R.S., Some consequences of thermo-solutal convection: The grain structure of castings. *Metall. Mater. Trans. A*, vol. 27A, pp. 569- 581 (1996).

Hellawell, A., "Modelling of casting, welding and advanced solidification processes." Eds. M. Cross and J. Campbell, *The Minerals, Metals & Materials Society*, Warrendale, PA, pp. 565-584, October 1995.

Hellawell, A., "Grain evolution in conventional and rheo-castings." *Proceedings of the 4th Int. Conf. On Semi-Solid Processing of Alloys and Composites*, Sheffield, England, pp. 60-65, June 1996.

Hofmeister, W.H., Bassler, B.T., and Bayuzick, R.J. "Measurement of High Speed Solidification Events." *International Symposia on Advanced Materials and Technology for the 21st Century*, The 117th Meeting of JIM, Honolulu, Hawaii, December 1995.

Holmes, D.E. "Dimensional Stability of Supermatrix Semiconductors." *Microgravity Materials Science Conference*, Huntsville, Alabama, June 10-11, 1996.

Huang, H.-W., Heinrich, J.C., and Poirier, D.R., Numerical anomalies in simulating directional solidification of binary alloys. *Numer. Heat Transfer, Part A*, (1996).

Huang, H.-W., Heinrich, J.C., and Poirier, D.R., Simulation of directional solidification with steep thermal gradients. *Model. Simul. Mater. Sci. Eng.*, (1996).

Hui, M., Beatty, K.M., Blackmore, K., and Jackson, K.A. "Impurity Distribution in InSb Single Crystals." *Tenth American Conference on Crystal Growth*, Vail, Colorado, August 6, 1996.

Isono, N., Smith, Patrick Michael, Turnbull, D., and Aziz, M.J. Anomalous diffusion of Fe in liquid Al measured by the pulsed laser technique. *Metallurgical and Materials Transactions A*, vol. 27, 725-730 (1996).

Isono, N., Smith, Patrick Michael, Turnbull, D., and Aziz, M.J. Anomalous diffusion of Fe in liquid Al measured by the pulsed laser technique. *Metallurgical and Materials Transactions A*, 27, 725-730 (1996).

Izmailov, A.F., and Myerson, A.S. Concentration Dependence of Solution Shear Viscosity and Solute Mass Diffusivity in Crystal Growth from Solutions. *Phys. Rev. E*, 52, 805 (1995).

Izmailov, A.F., and Myerson, A.S. Gravity Induced Formation of Concentration Gradients in Supersaturated Binary Solutions. *Physica*, vol. A 244, 503 (1996).

Izmailov, A.F., and Myerson, A.S. "Moment and Mass Transfer in Supersaturated Solutions and Its Consequences for Crystal Growth from Solutions." *The Tenth American Conference on Crystal Growth*, Vail, Colorado (1996).

Izmailov, A.F., Arnold, S., Holler, S., and Myerson, A.S. Microparticle driven by Parametric and Random Forces: Theory and Experiment. *Phys. Rev. E*, 52, 1325 (1995).

Izmailov, A.F., Myerson, A.S., and Na, H.S. Supersaturated Electrolyte Solutions: Theory and Experiment. *Phys. Rev. E*, 52, 4 (1995).

Izmailov, A.F., Myerson, A.S., and Na, H.S. Supersaturated Electrolyte Solutions: Theory and Experiment. *Phys. Rev. E*, vol. 52, 3923 (1995).

Izmailov, A.F., Myerson, A.S., and Na, H.S. "Supersaturated Electrolyte Solutions: Theory and Experiment." *American Institute of Chemical Engineers (AIChE) Annual Meeting*, Miami, Florida (1995).

Izmailov, A.F., Myerson, A.S., and Na, H.S. "Supersaturated Electrolyte Solutions: Theory and Experiment." *American Institute of Chemical Engineers (AIChE) Annual Meeting*, Miami, Florida (1995).

Izmailov, A.F., Myerson, A.S., Regel, L.L., and Wilcox, W.R. "Influence of High Gravity on Cluster Formation and Nucleation." *The Third International Workshop on Materials Processing at High Gravity*, Clarkson University, New York (1996).

Izmailov, A.F., Myerson, A.S., Regel, L.L., and Wilcox, W.R. "Influence of High Gravity on Cluster Formation and Nucleation." *46th International Astronautical Federation Congress*, Oslo, Norway (1995).

J. C. Westhoff, Model materials for vapor phase sintering in microgravity. M. S. Thesis, Colorado School of Mines, (January, 1996).

Jackson, K.A. "Monte Carlo Simulation Of Non-equilibrium Segregation During Crystal Growth." *Cornell University*, November 14, 1995.

Jackson, K.A. "Non-equilibrium Segregation During Crystallization." *Microgravity Materials Science Conference*, Huntsville, June 10-11, 1996.

Jackson, K.A. "Non-equilibrium Segregation During Crystallization." *Conference on Structural and Dynamic Modeling of Mechanical Behavior of Solids*, Monte Verita, Switzerland, September 5, 1996.

Jackson, K.A., Gilmer, G.H., and Temkin, D.E. Monte Carlo Simulation of the Rapid Crystallization of Bismuth-doped Silicon. *Phys. Rev. Letters*, vol. 75, 2530 (1995).

Jackson, K.A., Gilmer, G.H., Temkin, D.E., and Beatty, K.M. Microsegregation Far From Equilibrium. *J. Cryst. Growth*, vol. 163, 461 (1996).

Kane, D.B., and El-Shall, M.S. Condensation of supersaturated vapors of hydrogen bonding molecules: ethylene glycol, propylene glycol, trimethylene glycol and glycerol. *J. Chem. Phys.*, vol. 105, 7617-7632 (1996).

Kane, D.B., and El-Shall, M.S. Ion nucleation as a detector: application of REMPI to generate selected ions in supersaturated vapors. *Chem. Phys. Letters*, vol. 259, 482-487 (1996).

- Kane, D.B., Fisenko, S.P., and El-Shall, M.S. "Pressure effect on nucleation rate measurements in diffusion cloud chambers." Fourteenth International Conference on Nucleation and Atmospheric Aerosols, Helsinki, Finland, August 26-30, 1996.
- Karma, A., and Trivedi, R. "Role of Dynamics Nucleation at Moving Boundaries in Phase and Microstructure Selection." NASA Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.
- Kaschnitz, E., and Cezairliyan, A. Radiance Temperatures at 1500 nm of Niobium and Molybdenum at Their Melting Points by a Pulse-Heating Technique. *Int. J. Thermophys.*, vol. 17, 1069-1078 (1996).
- Kaschnitz, E., McClure, J., and Cezairliyan, A. "Radiance Temperatures (in the Wavelength Range 500-1500 nm) of Cobalt and Iron at Their Melting Points by a Pulse-Heating Technique." 14th European Conference on Thermophysical Properties, Lyon, France, September 1996.
- Kassemi, M., and Naraghi, M.N.H., "Application of discrete exchange factor method to combined heat transfer problems in cylindrical media." International Mechanical Engineering Congress and Exposition, November 1996.
- Kassemi, M., and Naraghi, M.N.H., "Interaction of radiation with conduction and convection in solidification of oxide crystals." Proceedings of the International Symposium on Radiative Heat Transfer, International Center for Heat and Mass Transfer, Begell House Inc., New York, 1996.
- Kassemi, M., Sayir, A., Farmer, S., and Chait, A. "Identification of Gravity-Related Effects on Crystal Growth from Melts with an Immiscibility Gap." The Third Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.
- Kaukler, W.K., and Curreri, P.A. "X-Ray Transmission Microscopy of Al-Pb Monotectic Alloys During Directional Solidification." Proceedings of the 8th International Symposium on Experimental Methods for Microgravity Materials Science, 125 TMS Annual Meeting, Anaheim, California, February 4-8, 1996.
- Kaukler, W.K., and Curreri, P.A. "Advancement of X-ray Microscopy Technology and its Application to Metal Solidification Studies." Proceedings of the 1996 SPIE Technical Conference in Space Processing of Materials, paper #5, pp 34-44, Proceedings Vol. 2809, N. Ramachandran, ed., August 4, 1996.
- Kelton, K.F. "Kinetic Analysis of Nonisothermal Crystallization (Invited Talk)." Proceedings of the Materials Research Society (MRS), Thermodynamics and Kinetics of Phase Transformations (J.S. Im, B. Park, A.L. Greer, and G.B. Stephenson, eds), vol. 398 (1995).
- Kelton, K.F. "Analysis of Crystallization Kinetics (Invited Talk)." Proceedings of the Ninth International Conference on Rapidly Quenched Metals, Bratislava, Slovakia (1996) (to appear in *Mat. Sci. and Eng.*).
- Kelton, K.F. "Nucleation (Invited Talk)." Proceedings of summer school: Phasenubergänge in Metallen, Institut für Raumsimulation, DLR, Cologne, Germany, June 4-5, 1996.
- Kelton, K.F. "Phase Formation and Stability: Composition and Sample-Size Effects." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.
- Kelton, K.F. "From Liquids to Crystals." Distinguished Lecture Series, Arkansas Tech University, Russellville, Arkansas, April 1996.
- Kelton, K.F., Lakshmi Narayan, K., Levine, L.E., Cull, T.C., and Ray, C.S. Computer Modeling of Nonisothermal Crystallization. *J. Non-Cryst. Solids*, (1996 in press).
- Kessel, A.R., Temnikov, A.N., Izmailov, A.F., and Myerson, A.S. "New and Effective Technique to study Supersaturated Solutions by the Pulsed (Spin-Echo) NMR Method." *Crystal Growth of Organic Materials*, ACS, Washington, D.C., p 266 (1996).
- Khan, A., and Pojman, J.A. "Frontal Polymerization of n-Butyl Acrylate." ACS National Meeting, New Orleans, Louisiana, March 24-28, 1996.
- Khan, A.M., and Pojman, J.A. The Use of Frontal Polymerization in Polymer Synthesis. *Trends in Polymer Science*, vol. 4, 253 (1996).

- Kim, G.T., Lin, J.T., Jones, O.C., Glicksman, M.F., Duval, W.M.B., Singh, N.B., Effects of convection during the physical vapor transport process: application of laser doppler velocimetry. *Journal of Crystal Growth*, (in press, 1996).
- Konagurthu, S., Krantz, W.B., Greenberg, A.R., and Todd, P. "A Novel Approach to Test Alternative Hypotheses for Macrovoid Growth in Polymeric Membranes." Eighth Annual Meeting of the North American Membrane Society, Ottawa, Canada, May 1996 (the NAMS technical committee awarded first place for the best student paper).
- Korpela, S., Chait, A., and Kassemi, M., Radiative heat transfer in fiber drawing and crystal pulling. *Journal of Crystal Growth*, (1996).
- Kurtze, D.A., Noise and dynamical pattern selection. *Phys. Rev. Lett.*, 77, 63 (1996).
- Kyrilidis, A. and Brown, R.A. Density functional theory of melt-solid interfaces in hard sphere systems. *Physical Review E*, 51, 5832-5845 (1995).
- Lakshmi Narayan, K., and Kelton, K.F. "Composition Effects on Nucleation and Growth in $\text{Na}_2\text{O}_2\text{CaO}_3\text{SiO}_2$ glasses." Mid-West Solid State Conference, St. Louis, Missouri, October 1996.
- Lakshmi Narayan, K., and Kelton, K.F. "Crystallization Behavior in $\text{Na}_2\text{O}_2\text{CaO}_3\text{SiO}_2$ Glasses." Meeting of the American Physical Society, St. Louis, Missouri, April 1996.
- Lakshmi Narayan, K., Kelton, K.F., and Ray, C.S. Effect of Pt Doping on Nucleation and Crystallization in $\text{Li}_2\text{O} \cdot 2\text{SiO}_2$ Glass: Experimental Measurements and Computer Modeling. *J. Non-Cryst. Solids*, vol. 195, 148-157 (1996).
- Lantz, C., Teft, P., Moore, J.J., and Readey, D.W., "Self propagating reactive synthesis of ceramics in a microgravity environments." TMS Symposium "Experimental Methods for Microgravity Materials Science", Eds: R. Schifman, C. Patielli, pub. by TMS, pp. 41-44, October 1995.
- Larson Jr., D.J., Dudley, M., Chung, H., and Raghothamachar, B. "Synchrotron Characterization of Zn-Alloyed CdTe Compound Semiconductors Processed in Microgravity on STS-50 and STS-73." *IUCR Proceedings* (1996).
- Levine, L.E., Narayan, K.L., and Kelton, K.F. Finite size corrections for the Johnson-Mehl-Avrami-Kolmogorov Equation. *J. Mater. Res.*, (1996 in press).
- Li, B.Q., and de Groh, H.C. "Study of Magnetic Damping Effect on Convection and Solidification under G-Jitter Conditions (poster presentation)." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.
- Lin, C. and Witt, A.F. New approaches to growth and characterization of photo-refractive BSO (Bi_2SiO_2). *J. Crystal Growth*, (accepted, 1996).
- Mackowski, D.W., and Knight, R.W. Numerical investigation of thermal creep and thermal stress effects in microgravity physical vapor transport, Final Technical Report for NASA contract NAG8-977. Auburn University, Department of Mechanical Engineering, (January 1996).
- Mackowski, D.W., and Knight, R.W. "Investigation of thermal stress convection in nonisothermal gases under microgravity conditions." Third Microgravity Fluid Physics Conference, Cleveland, Ohio, June 1996 (NASA Conference Publication 3338).
- Mackowski, D.W., Rao, V.R., and Knight, R.W. Effect of solid phase heat transfer and wall deposition on crystal growth in physical vapor transport ampoules. *J. of Cryst. Growth*, vol. 165, 323-334 (1996).
- Mallika, C., Narayanan, R., and Anderson, T.J. "Modeling of Fluid Flow Occurring During the Measurement of Diffusivity in Liquid Metals." Second Fluids in Space Conference, Naples, Italy, May 1996.
- Mani, S.S., Singh, N.B., Coriell, S.R., Glicksman, M.E., and Duval, W.M.B. "In situ Observations of interface instability During Growth of Lead Bromide Crystals." Proceedings of "Materials Research Society, Optoelectronic Materials, Ordering Composition, Modules and self Assembled Structures" (E.D. Jones, A. Mascarenhas, and P. Petroff,
- Mathias, L.J., Thigpen, K.T., and Avci, D. Superfast Methacrylate Photomonomers: Aryl Ester Derivatives of Ethyl α -Hydroxymethacrylates. *Macromolecules*, vol. 28, 8872 (1995).

- Mayer, S., and Ostrogorsky, A.G. "Forced Convection in Vertical Bridgman Configuration with the Submerged Heater." Tenth American Crystal Growth Conference, Vail, Colorado, August 1996.
- Mehrabi, M.R. and Brown, R.A. Parallel implementation of finite-element/Newton method for solution of steady-state and transient nonlinear partial differential equations. *J. Sci. Computing*, 10, 93-137 (1995).
- Meyer, S., and Ostrogorsky, A.G. Interface Shape and Segregation in Vertical Bridgman Configuration with and without the Submerged Heater. *J. Crystal Growth*, (in print).
- Meyer, S., and Ostrogorsky, A.G. Forced Convection in Vertical Bridgman Configuration with the Submerged Heater. *J. Crystal Growth*, (in print).
- Myerson, A.S., and Izmailov, A.F. "Study of Organic Supersaturated Solution: Theory and Experiment." *Crystal Growth of Organic Materials*, ACS, Washington, D.C., p 222 (1996).
- Myerson, A.S., and Izmailov, A.F. "Thermodynamic Properties of Supersaturated Electrolyte Solutions." The 13th Symposium on Industrial Crystallization, Toulouse, France (1996).
- Myerson, A.S., and Izmailov, A.F. "Fluctuation-Dissipation Theorem for Supersaturated Electrolyte Solutions." The Tenth American Conference on Crystal Growth, Vail, Colorado (1996).
- Myerson, A.S., and Izmailov, A.F. "Study of Organic Supersaturated Solution: Theory and Experiment." *Crystal Growth of Organic Materials*, ACS, Washington, D.C., p 222 (1996).
- Myerson, A.S., and Izmailov, A.F. "Thermodynamic Properties of Supersaturated Electrolyte Solutions." The 13th Symposium on Industrial Crystallization, Toulouse, France (1996).
- Myerson, A.S., and Izmailov, A.F. "Fluctuation-Dissipation Theorem for Supersaturated Electrolyte Solutions." The Tenth American Conference on Crystal Growth, Vail, Colorado (1996).
- Ostrogorsky, A.G. "Solidification by the Submerged Heater Method." Centre d'Etudes Nucleaires in Grenoble, France, May 1996.
- Paley, M.S. "Photodeposition of Polydiacetylene Thin Films for Photonic Applications in 1-g and in Microgravity." SPIE Conference, Denver, Colorado, August 1996.
- Paley, M.S., and Frazier, D.O. "Photodeposition of Polydiacetylene Thin Films for Photonic Applications in 1-g and in Microgravity." *SPIE Proceedings*, Denver Colorado, August 1996, vol. 2809, p 114.
- Paley, M.S., Armstrong, S., Witherow, W.K., and Frazier, D.O. Kinetic Studies on Photodeposition of Polydiacetylene Thin Films from Solution: Preliminary Determination of the Rate Law. *Chem. Mater.*, vol. 8, no. 4, 912 (1996).
- Palosz, W. "Removal of oxygen from electronic materials by vapor phase processes." ACCG-10/ICVGE-9, Vail, Colorado, August 1996.
- Palosz, W. "Investigation of convective effects in crystal growth by PVT." Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.
- Palosz, W., Gillies, D., Grasza, K., Chung, H., Raghothamachar, B., and Dudley, M. "Characterization of cadmium-zinc telluride crystals grown by "contactless" PVT using synchrotron topography." ACCG-10/ICVGE-9, Vail, Colorado, August 1996.
- Papa Rao, S.S. Control of the growth interface location in vertical Bridgman geometry (PhD Thesis, MIT). (1996).
- Papa Rao, S.S. and Witt, A.F. Control of growth interface location and morphology in a heatpipe-based vertical Bridgman system. *J. Crystal Growth*, (accepted, 1996).
- Pascal, L., and Gokhale, A.M., Computer simulation of spatial arrangement and connectivity of features in three-dimensional microstructure: application to model electrical conductivity of polymer matrix composite. *Acta Metallurgica et Materialia*, vol. 44, pp 1519-1528 (1996).

- Perepezko, J.H. "Analysis of Containerless Processing and Undercooled Solidification Microstructures." Microgravity and Materials Science DWG Meeting, Huntsville, Alabama, June 1996.
- Perepezko, J.H. "Analysis of containerless processing and undercooled solidification microstructures ." Microgravity and Materials Science DWG Meeting, Huntsville, AL, June, 1996.
- Perepezko, J.H. and Allen, D.R. "Kinetic competition in undercooled liquid alloys." Thermodynamics and Kinetics of Phase Transformations 398, Proceedings of the Materials Research Society Symposium, J.S. Im, B. Park, A.L. Greer, and G.B. Stephenson eds., 3 (1996).
- Perepezko, J.H. and Allen, D.R. "Kinetic competition in undercooled liquid alloys." Materials Research Society Fall Meeting, Boston, MA, November, 1995.
- Pilling, J., and Hellawell, A., Mechanical deformation of dendrites by fluid flow. Metall. Mater. Trans. A., vol. 27A, pp. 229-232 (1996).
- Pojman, J.A. "Frontal Polymerization: Quo Vadis?" ACS National Meeting, New Orleans, Louisiana, March 24-28, 1996.
- Pojman, J.A. "Frontal Polymerization: From Dynamics to Materials (invited presentation)." 28th Congress National D'Analyse Numerique, La Londe-Les Maures, France, May 29, 1996.
- Pojman, J.A., and Khan, A. "Reactor Design and Performance for the Study of Frontal Polymerization." ACS National Meeting, Orlando, Florida, August 25-29, 1996.
- Pojman, J.A., Fortenberry, D., Khan, A., and Ilyashenko, V.M. "Frontal Polymerization: Self-Propagating High Temperature Synthesis (SHS) of Polymeric Materials." ACS National Meeting, Orlando, Florida, August 25-29, 1996.
- Pojman, J.A., Gilla, N., Willis, J., and Whitehead, J.B. "Polymer Dispersed Liquid Crystal (PDLC) Materials Produced via Frontal Epoxy Curing." ACS National Meeting, Orlando, Florida, August 25-29, 1996.
- Pojman, J.A., Ilyashenko, V.M., and Khan, A. Free-Radical Frontal Polymerization: Self-Propagating Thermal Reaction Waves. J. Chem. Soc., Faraday Trans., vol. 92, 2824 (1996).
- Popov, D.I., Regel, L.L., and Wilcox, W.R. "Numerical modeling of detached solidification." American Conference on Crystal Growth - 10, Vail, Colorado (July 1996).
- Popov, D.I., Regel, L.L., and Wilcox, W.R. "Numerical Modeling of Detached Solidification." 70th Colloid and Surface Science Symposium, Clarkson University (June 1996).
- Prasad, S., Mallika, C., Narayanan, R., and Anderson, T.J. "A Novel Flow Visualization Technique for the Determination of Dynamic States in a Bridgman Crystal Growth Configuration." AIAA 96-0255, 34th AIAA National Meeting.
- Qui, N., and Apfel, R. Rapid decompression of seeded melts for materials processing. Rev. Sci. Instrum., vol. 65, 3337-3343 (1995).
- Ray, C.S., Day, D.E., Huang, W., Lakshmi Narayan, K., Cull, T.S., and Kelton, K.F. Nonisothermal Calorimetric Studies of the Crystallization of Lithium Disilicate Glass. J. Non-Cryst. Solids, (1996 in press).
- Readey, D.W., Aldrich, D.J., and Ritland, M.A., Vapor transport and sintering. Sintering Technology, R.M. German, G.L. Messing, and R.G. Cornwall, eds., (Marcel Dekker, NY), pp. 53-60 (1996).
- Readey, D.W., Aldrich, D.J. and Westhoff, J.H., "Vapor phase sintering." Poster Presentation at the NASA Microgravity Materials Science Meeting, Huntsville, AL, June 1996.
- Readey, D.W. and Ritland, M.A., Reactive vapor phase sintering for the production of porous materials and composites. Processing and Fabrication of Advanced Materials IV, T.S. Srivatsan and J.J. Moore, eds., (TMS, Warrendale, Pa.), pp. 151-164 (1996).
- Reddy, K.S.N., Salvati, L.M., Dutta, P.K., Abel, P.B., Suh, K.I., and Ansari, R.R. Reverse Micelle Based Growth of Zincophosphate Sodalite: Examination of Crystal Growth. J. of Physical Chem., vol. 100, 9870-9880 (1996).

- Reddy, K.S.N., Salvati, L.M., Dutta, P.K., Abel, P.B., Suh, K.I., and Ansari, R.R., Reverse micelle based growth of zincophosphate sodalite: examination of crystal growth. *Journal of Physical Chemistry*, 100, 9870-9880 (1996).
- Regel, L.L., Popov, D.I., and Wilcox, W.R. "Detached solidification: Steady state results." *Proceedings of the Microgravity Materials Science Conference*, Huntsville, Alabama (June 1996).
- Regel, L.L., Popov, D.I., and Wilcox, W.R. "Modeling of detached solidification." *IAF Congress*, Oslo, Norway (October 1995).
- Rhim, W.-K. "Thermophysical Property Measurement of Molten Semiconductors in 1-g and Reduced-g Conditions (poster presentation)." *Microgravity Materials Science Conference*, Huntsville, Alabama, June 10-11, 1996.
- Rhim, W.-K. "Undercooling Limits and Thermophysical Properties in Glass Forming Alloys (poster presentation)." *Microgravity Materials Science Conference*, Huntsville, Alabama, June 10-11, 1996.
- Schwenke, G.K. "Analysis of the Non-Isothermal Impaction Spreading and Freezing of Metal Droplets." MIT MS Thesis (June 1996).
- Sen, S., Dhindaw, B.K., Stefanescu, D.M., and Curreri, P.A. Melt Convection Effects on the Critical Velocity of Particle Engulfment. *J. of Crystal Growth*, (August 1996, accepted).
- Sen, S., Dhindaw, B.K., Stefanescu, D.M., and Curreri, P.A. "Melt Convection Effects on the Critical Velocity of Engulfment in the Biphenyl/Glass Particles system." *Proceedings of the 8th International Symposium on Experimental Methods for Microgravity Materials Science*, 125 TMS Annual Meeting, Anaheim, California, February 4-8, 1996.
- Shao, Y., and Spaepen, F. Undercooling of bulk liquid silicon in an oxide flux. *J. of Applied Physics*, vol. 79, 2981-2985 (1996).
- Shao, Y. and Spaepen, F. Undercooling of bulk liquid silicon in an oxide flux. *Journal of Applied Physics*, 79, 2981-2985 (1996).
- Shen, X.F., Anilkumar, A.V., Grugel, R.N., and Wang, T.G. Utilizing vibration to promote microstructural homogeneity during floating-zone crystal growth processing. *J. Cryst. Growth*, vol. 165, 438-446 (1996).
- Singh, N.B. "Assessing the Crystal Growth and Operating Characteristics of Acousto-Optical Materials." Anna University, Madras, India, January 28-30, 1996.
- Singh, N.B., Coriell, S.R., Mani, S.S., Glicksman, M.E., and Duval, W.M.B. "Flight Experiment to Study Double Diffusive Instabilities in Silver doped Lead Bromide Crystals." *Microgravity Materials Science Conference*, Huntsville, Alabama, June 10-12, 1996.
- Singh, N.B., Glicksman, M.F., Coriell, S.R., Duval, W.M.B., Santoro, G.J., Dewitt, R., Measurement of diffusion coefficient using a diaphragm cell: PbBr₂-AgBr. *Journal of Crystal Growth*, (in press, 1996).
- Singh, N.B., Mani, S.S., Adam, J.D., Coriell, S.R., Glicksman, M.E., Duval, W.M.B., Santoro, G.J., and DeWitt, R. Direct Observations of Instabilities. *J. Crystal Growth*, vol. 166, 364 (1996).
- Slepicka, J.S., and Cha, S.S. "Holographic Diffraction Image Velocimetry for the Measurement of Three-Dimensional Velocity Fields." AIAA-96-2265, presented at the 19th AIAA Advanced Measurement and Ground Testing Technology Conference, New Orleans, Louisiana, June 1996.
- Song, H., Tewari, S.N., and de Groh III, H.C., Convection during thermally unstable solidification of Pb-Sn in a magnetic field. *Met. and Mat. Trans. A*, vol. 27A, pp. 1095-1110. (April 1996).
- Spaepen, F. "Measurements of Interface Stress and Interfacial Enthalpy." *Materials Research Society Fall Meeting, Symposium on Metastable Metal-Based Phases and Microstructures*, Boston, Massachusetts, November 1995.
- Spaepen, F. "The Temperature Dependence of the Crystal-Melt Interfacial Tension." *Materials Research Society Fall Meeting, Symposium on Thermodynamics and Kinetics of Phase Transformations*, Boston, Massachusetts, November 1995.

- Spaepen, F. "Kinetics of Nucleation and Growth From Undercooled Melts." Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.
- Spaepen, F. "The interface between a crystal and its melt: Structure, tension, and implications for nucleation." Materials Science Colloquium, University of Virginia, Charlottesville, Virginia, October 1995.
- Spaepen, F. "The interface between a crystal and its melt: structure, tension, and implications for nucleation." Department of Mechanical Engineering, Yale University, New Haven, Connecticut, February 1996.
- Spaepen, F. "Structure and thermodynamics of interfaces." DeVivio Lecture in Materials Science, Northeastern University, Boston, Massachusetts, March 1996.
- Spaepen, F. "Effect of structural non-uniformity on the temperature dependence of the crystal-melt interfacial tension." Ninth International Conference on Rapidly Quenched and Metastable Materials, Bratislava, Slovakia, August 1996.
- Spaepen, F. "Measurements of interface stress and interfacial enthalpy." Materials Research Society Fall Meeting, Symposium on Metastable Metal-Based Phases and Microstructures, Boston, Massachusetts, November 1995.
- Spaepen, F. "The temperature dependence of the crystal-melt interfacial tension." Symposium on Thermodynamics and Kinetics of Phase Transformations, Boston, MA, November, 1995.
- Spaepen, F. "Key Invitee and Rapporteur." ARPA/NSF Workshop on Modeling of Film Growth and Deposition Processes Q Evolution of Film Microstructure and Morphology, Institute for Mathematics and Its Applications, University of Minnesota, Minneapolis, Minnesota, January 1996.
- Spaepen, F. "Kinetics of nucleation and growth from undercooled melts." Microgravity Materials Science Conference, Marshall Space Flight Center, Huntsville, Alabama, June 1996.
- Spaepen, F. "The interface between a crystal and its melt: Structure, tension, and implications for nucleation." Materials Science Colloquium, University of Virginia, Charlottesville, Virginia, October 1995.
- Spaepen, F. "The interface between a crystal and its melt: structure, tension, and implications for nucleation." Department of Mechanical Engineering, Yale University, New Haven, Connecticut, February 1996.
- Spaepen, F. "Effect of structural non-uniformity on the temperature dependence of the crystal-melt interfacial tension." Ninth International Conference on Rapidly Quenched and Metastable Materials, Bratislava, Slovakia, August 1996.
- Spaepen, F., and Shao, Y. "The crystal-melt interface in Si or Ge." Materials Research Society Symposium Proceedings, 398, 39-44 (1996).
- Spaepen, F. and Shao, Y. "The crystal-melt interface in Si or Ge." Materials Research Society Symposium Proceedings, 398, 39-44 (1996).
- Spaepen, F. (Key Invitee and Rapporteur) "Evolution of Film Microstructure and Morphology." ARPA/NSF Workshop on Modeling of Film Growth and Deposition Processes, Institute for Mathematics and Its Applications, University of Minnesota, Minneapolis, Minnesota, January 1996.
- Stefanescu, D.M., Leon-Torees, J., Sen, S., and Dhindaw, B.K. "Influence of gravitational acceleration on the macrosegregation of Al-Cu alloys." 3rd International Conference on Modeling of Casting and Solidification Processes, Beijing, China, December 1996.
- Szofran, F.R. "Magnetic damping of solid solution semiconductor alloys." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.
- Szofran, F.R., Motakef, S., and Volz, M.P. "Bridgman growth of Ge:Ga in a static magnetic field." Presented at the Tenth American Conference on Crystal Growth, Vail Colorado, August, 1996.
- Tewari, A., and Gokhale, A.M. "Evolution of Microstructural Distance Distributions During Liquid Phase Sintering in Normal Gravity and Microgravity." NASA Microgravity Materials Science Conference, Huntsville, Alabama, June 10-12, 1996.

- Tewari, A. and Gokhale, A.M., "Evolution of microstructural distance distributions during liquid phase sintering in normal gravity and microgravity." Microgravity Materials Science Conference, organized by NASA., Huntsville, Alabama, June 10-12, 1996.
- Tewari, S.N., and Shah, R., Macrosegregation during dendritic arrayed growth of hypoeutectic Pb-Sn alloys: Influence of primary arm spacing and mushy zone length. *Metall. Mater. Trans. A*, (1996).
- Trolinger, J.D., Lal, R.B., McIntosh, D., and Witherow, W.K. Holographic Particle Image Velocimetry in the First International Microgravity Laboratory aboard the Space Shuttle Discovery. *Applied Optics*, vol. 35, no. 4, 681-689 (1996).
- Trolinger, J.D., Rangel, R., and Lal, R. "Particle Mechanics and G-jitter Observations in the IML-1 Spaceflight." AIAA 96-0504, 34th Aerospace Sciences Meeting, January 1996.
- Tryggvason, G., Ceccio, S.L., and Jacqmin, D., "Fundamentals of mold free casting: experimental and computational studies." *Microgravity Science and Applications*, NASA Technical Memorandum 4735, p. 724, 1996.
- Tryggvason, G., Ceccio, S. L. and Jacqmin, D., Fundamentals of mold free casting: experimental and computational studies. *NASA Tech Brief*, 4735, p. 724 (1996).
- Tryggvason, G., Juric, D., Han, J., and Ceccio, S.L., "Direct numerical simulations in material processing." in *Space Processing of Materials*, Narayanan Ramachandran, Editor, Proc. SPIE 2809, 178-184, 1996.
- Tryggvason, G., Juric, D., Han, J. and Ceccio, S.L., "Direct numerical simulations in material processing." in *Space Processing of Materials*, Narayanan Ramachandran, Editor, Proc. SPIE 2809, pp. 178-184 (1996).
- Varanasi, C., Black, M.A., and McGinn, P.J. The Demonstration of Y_2BaCuO_3 Particle Segregation in Melt Processed $YBa_2Cu_3O_x$ Through a Computer Visualization Model. *J. Materials Research*, vol. 11, 565-571 (1996).
- Volz, M.P., and Mazuruk, K. Flow transitions in a rotating magnetic field. *Experiments in Fluids*, vol. 20, 454-459 (1996).
- Volz, M.P., and Mazuruk, K. "Damping of natural convection in liquid gallium with a rotating magnetic field." Tenth American Conference on Crystal Growth, Vail, Colorado, August 1996.
- Wang, C.Y. and Beckermann, C., Equiaxed dendritic solidification with convection: Part 1, multi-scale/-phase modeling. *Met. and Mat. Trans.*, (1996).
- Wang, C.Y. and Beckermann, C., Equiaxed dendritic solidification with convection: Part 2, numerical simulations for an Al-4wt%Cu alloy. *Met. and Mat. Trans.*, (1996).
- Wang, C.Y. and Beckermann, C., Equiaxed dendritic solidification with convection: Part 3, comparisons with NH_4Cl-H_2O experiments. *Met. and Mat. Trans.*, (1996).
- Weber, J.K.R. "Containerless Property Measurements on Molten Aluminum Oxide and Alumino-Silicate Binary Mixtures." Proc. 4th Asian Thermophysical Properties Conference, Tokyo, Japan, September 5-8, 1995, A. Nagashima, ed., pp 873-876.
- Weber, J.K.R. "From Basic Research to Applied Materials - Containerless Liquid-Phase Processing of Molten Oxides." Department of Materials Science Research Seminar, University of Illinois at Urbana-Champaign, Champaign, Illinois, September 19, 1996.
- Weber, J.K.R., and Nordine, P.C. Containerless Liquid-Phase Processing at High temperatures. *Microgravity Science and Technology*, vol. VII, 279-282 (1995).
- Weber, J.K.R., and Nordine, P.C. "Process-Property-Structure Relationships in Complex Oxide Melts." NASA Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.
- Weber, J.K.R., Anderson, C.D., Krishnan, S., and Nordine, P.C. Structure of Aluminum Oxide Formed from Undercooled Melts. *J. Am. Ceram. Soc.*, vol. 78, 577-582 (1995).

- Weber, J.K.R., Felten, J.J., and Nordine, P.C. New Method for High Purity Ceramic Synthesis. *Rev. Sci. Instrum.*, vol. 67, 522-524 (1996).
- Weber, J.K.R., Felten, J.J., Cho, B., and Nordine, P.C. Design and Performance of the Aero-Acoustic Levitator. *J. Jpn. Soc. Microgravity Appl.*, vol. 13, 27-35 (1996).
- Weber, J.K.R., Felten, J.J., Cho, B., Lockwood, N., and Nordine, P.C. "New Observations of Undercooled Oxide Solidification." Gordon Research Conference on High Temperature Chemistry, Tilton School, Tilton, New Hampshire, July 23, 1996.
- Weber, J.K.R., Krishnan, S., and Nordine, P.C. Effects of Melt Chemistry on the Spectral Absorption Coefficient of Liquid Aluminum Oxide. *J. Am. Ceram. Soc.*, vol. 78, 3067-3071 (1995).
- Westhoff, J. H., and Readey, D.W., "Model materials for vapor phase sintering in microgravity." American Ceramic Society Annual Meeting, Indianapolis, IN, May 1996.
- Wilcox, W.R., and Regel, L.L. Detached solidification. *Microgravity Science and Technology*, vol. 8, 56-61 (1995).
- Wilcox, W.R., and Regel, L.L. "Influence of Convection on the Microstructure of Fibrous Eutectics." American Conference on Crystal Growth - 10, Vail, Colorado, July 1996.
- Wilcox, W.R., Regel, L.L., and Smith, R.W. "Use of Microgravity to Control the Microstructure of Eutectics." Microgravity Materials Science Conference, Huntsville, Alabama, June 10-11, 1996.
- Witt, A.F. and Presinger, A. "An initiative for European collaboration in crystal growth research and technology development." BMFW, Vienna, Austria (1995).
- Xia, Y. and Brown, R.A. Measurement of the onset of two-dimensional cellular solidification in the succinonitrile-acetone binary alloy. *J. Crystal Growth*, 154, 205-210 (1995).
- Yao, M., Chait, A., Fripp, A.L., and Debnam, W.J. Numerical Simulation of Bridgman Crystal Growth of PbSnTe in Microgravity. *Microgravity Science and Technology*, vol. 8, 214 (1995).
- Zeisler-Mashl, K.L., and Lograsso, T.L. Determination of the In-rich peritectic region in the In-Sn system by differential scanning calorimetry. *J. Phase Equilibria*, vol. 16, 516-519 (1995).
- Zeisler-Mashl, K.L., and Lograsso, T.L. Measurement of the peritectic phase composition in the Sn-Cd system through directional solidification techniques. *J. Phase Equilibria*, vol. 17, 7-9 (1996).
- Zeisler-Mashl, K.L., and Lograsso, T.L. "Band formation during directional solidification in peritectic systems." 1995 TMS Fall Meeting, Cleveland, Ohio, October 1995.
- Zeisler-Mashl, K.L., and Lograsso, T.L. "Microstructural development during directional solidification of peritectic alloys." Microgravity Materials Science Conference, Huntsville, Alabama, June 1996.
- Zeisler-Mashl, K.L., Lograsso, T.L., and Trivedi, R.K. "The influence of convection on banding in peritectic systems: a comparison of Sn-Cd and Pb-Bi." 8th International Symposium on Experimental Methods for Microgravity Materials Science, Anaheim, California, February 1996.
- Zhou, A., Zebis, A., Trivedi, S., Duval, W.M.B., Physical vapor transport of zinc-telluride by dissociative sublimation. *Journal of Crystal Growth*, (in press, 1996).

Advanced Technology Development

- Chave, R.G. Magnetostrictive Lead Screw Driver for Optics Positioning at Liquid Helium Temperature. NASA Tech Brief, JPL New Technology Report, (1996).
- Chave, R.G., Wiseman, T.A.J., Barnatz, M.B., and Hahn, I. "A Facility for Interferometric Measurement of Linear Displacement in Actuators and Calibration of Sensors at Cryogenic Temperatures Between 4.2 K and 77 K." SPIE 2865-10, SPIE Annual Meeting, Denver, 1996.

- Cheung, H.M., Meyer, W.V., Taylor, T.W., Tin, P., Barmatz, M.B., Biswas, A., Mann, J.A., Jr. "Hardware and software modifications of a commercial laser vibrometer for investigation of high amplitude surface fluctuations with optical tracking." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.
- Fultz, R., Chave, R.G., Birsan, M., and Barmatz, M.B. "New Polycrystalline Materials for Low Temperature Actuators in Space Science Instruments." Proposal to the President's Discretionary Fund Caltech, 1996.
- Greenberg, P., NASA tech brief: pulsed laser shot counter. NASA Tech Brief, (1996).
- Greenberg, P. and Ku, J. "Soot volume fraction imaging." Twenty-Sixth International Symposium on Combustion, Naples, Italy, July 28 - August 1, 1996.
- Greenberg, P.S., "Challenges and Capabilities of Microgravity Combustion Diagnostics." The Third International Workshop on Short-Term Experiments Under Strongly Reduced Gravity Conditions, Bremen, Germany, July, 1996.
- Greenberg, P. S., and Ku, J. C., Soot volume fraction imaging. Applied Optics, (1996).
- Lant, C.T., Smart, A.E., Cannell, D.S., Meyer, W.V., Doherty, M.P., "The physics of hard spheres experiment - a general purpose light scattering experiment." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.
- Mann, J.A., Jr., Farukhi, Z.H., "Surface laser light scattering: data processing and foundations." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.
- Meyer, W.V., Lock, J.A., Cannell, D.S. Taylor, T.W., Tin, P., Smart, A.E., Zhu, J.X., Cheung, H.M., Mann, J.A., Jr., "A single wavelength cross-correlation technique which suppresses multiple scattering." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.
- Ovryn, B., Andrews, J.H., and Eppell, S., "Phase-measuring laser feedback interferometry: applications to microscopy." SPIE Vol. 2655, pp 153-163, 1996.
- Ovryn, B., Andrews, J.H., Eppell, S., and Khaydarov, J., "Phase-shifted, real-time laser feedback interferometry." SPIE Vol. 2860, pp 263-275, 1996.
- Ovryn, B., Eppell, S.J., Andrews, J.H., and Khaydarov, J., "Application of phase shifted, laser feedback interferometry to fluid physics." Proceedings of the Third Annual Microgravity Fluids Conference, Cleveland, Ohio, June 1996.
- Proceedings: Moir, C.I., Greenberg, P.S., and MacGregor, A., "Compact laser velocimeter module." OSA Meeting on Photon Correlation, Capri, Italy, August, 1996.
- Rogers, R.B., Meyer, W.V., Zhu, J.X., Turner, W., Chaikin, P.M., Russel, W.B., "A compact laser light scattering instrument for microgravity research." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.
- Taylor, T.W., Meyer, W.V., Tin, P., Mann, J.A., Jr., Cheung, H.M., Rogers, R.B., Lading, L., "A new surface light scattering instrument with auto-tracking optics." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.
- Tin, P., Meyer, W.V., Rogers, R.B., Mann, J.A., Jr., Cheung, H.M., Taylor, T.W., "Fiber-Optics surface light scattering spectrometer (FOSLSS)." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.
- Tseng, C.S., Meyer, W.V., Tin, P., de Mul, M., Lando, J.B., Mann, J.A., Jr., "Laser light scattering spectroscopy combined with Brewster Angle Microscopy: nCB and polymer monolayers." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.
- Patent Approved, U. S. Patent #: Undetermined
- Vander Wal, R.L., "A patent application entitled "Laser processing of nanophase material" based on morphological changes observed in the laser-heated soot was submitted January 1995."
- Vander Wal, R. L., Laser-induced incandescence measurements of soot concentration in post-combustion exhaust. NASA Tech Brief, (Laser-Tech Briefs, accepted 1996).

- Vander Wal, R. L., Visualization of polycyclic aromatic hydrocarbons and soot via laser-induced excitation. NASA Tech Brief, (Laser-Tech Briefs, accepted 1996).
- Vander Wal, R. L., Soot visualization via laser-induced incandescence. NASA Tech Brief, (Laser Tech. Briefs 1996).
- Vander Wal, R. L., Soot precursor material: visualization via simultaneous LIF-LII and characterization via TEM. 26th Comb. Symp., (accepted 1996).
- Vander Wal, R.L., Laser-induced incandescence: detection issues. Applied Optics, (in press, 1996).
- Vander Wal, R.L., Identification of soot precursor material via simultaneous LIF-LII and characterization via TEM. Combustion Science and Technology, (accepted 1996).
- Vander Wal, R.L., "Laser-induced incandescence: characterization and applications ." 26th Symposium on Combustion, Naples Italy, July 28 - August 2, 1996.
- Vander Wal, R.L., "Laser-induced incandescence: detection issues." Central States Section Meeting of the Combustion Institute, St. Louis MO, May 5-7, 1996.
- Vander Wal, R.L., "Soot precursor material: location via LIF-LII and characterization via TEM." Central States Section Meeting of the Combustion Institute, St. Louis MO, May 5-7, 1996.
- Vander Wal, R.L. and Dietrich, D.L., Laser-induced incandescence applied to droplet combustion. Applied Optics, 34, pp. 1103-1107 (November 1995).
- Vander Wal, R.L., Jensen, K.A., and Choi, M.Y., Laser-induced emission measurements of soot and polycyclic aromatic hydrocarbons within a gas-jet flame. Combustion and Flame, (accepted 1996).
- Vander Wal, R.L., Jensen, K.A., Zhou, Z., and Choi, M.Y., "Soot precursor particles and polycyclic aromatic hydrocarbons: visualization through simultaneous laser-induced incandescence and laser-induced fluorescence imaging in diffusion flames." Eastern States Section Meeting of the Combustion Institute, Worcester MA, October 16-18, 1995.
- Vander Wal, R. L., Zhou, Z., and Choi, M. Y., Laser-induced incandescence calibration via gravimetric sampling. Combustion and Flame, (in press).
- Zhu, J.X., Chaikin, P.M., Li, M., Russel, W.B., Meyer, W.V., Rogers, W.V., "The structure and dynamics of hard sphere colloidal crystals under micro-gravity with quasi-elastic light scattering." Photon Correlation and Scattering OSA Meeting, Capri, August 21-25, 1996.

Technology Transfer

- Carter, D.C. "Progress in the Utilization of Polycapillary X-ray Optics for Application in Macromolecular Crystallography." Gordon Research Conference, New Hampshire, June 1996.
- Owens, S.M., Ullrich, J.B., Ponomarev, I.-Yu., Carter, D.C., Sisk, R.C., Ho, J.X., and Gibson, W.M. "Protein crystal structure measurements using polycapillary x-ray optics." SPIE Proceedings, vol. 2859-44, 1996.
- Ullrich, J.B., Huang, K.G., Owens, S.M., Aloisi, D.C., Hofmann, F.A., Gao, N., Klotzko, I.L., and Gibson, W.M. Concentration of synchrotron beams by means of monolithic polycapillary X-ray optics. Nucl. Inst. and Meth., vol. A364, 362 (1995).
- Ulrich, J., Owens, S.M., Xiao, Q.-F., Ponomarev, I.-Yu., Carter, D.C., Sisk, R.C., and Gibson, W.M. "Convergent Beam Macromolecular Crystallography using Polycapillary X-ray Optics." International Union of Crystallography, Seattle, Washington, August 1996.

Appendix

A	Table of Acronyms	A-1
B	Guest Investigator Index	B-1
C	Principal Investigator Index	C-1

The following list of acronyms, though by no means complete, includes those used in this document as well as some that are often found in text associated with Microgravity Science and Applications research and which may be encountered when reviewing references cited in the bibliography herein.

3AAL	Three-Axis Acoustic Levitator
3M	Minnesota Mining and Manufacturing Company
A	Ampere
A&R	Automation and Robotics
AADSF	Advanced Automated Directional Solidification Furnace
AAL	Aero-acoustic Levitation
AC&S	Altitude Control and Stabilization
ACA	Attitude Control Assembly
ACC	Aft Cargo Carrier
ACCG	American Conferences of Crystal Growers
ACES	Acoustic Containerless Experiment System
ACPF	Acoustic Containerless Processing Facility
ACRT	Accelerated Crucible Rotation Technique
ACS	Attitude Control System
ADA	Advanced Development Activity
ADA	DOD High-Level Programming Language
ADH	Advanced Development Hardware
ADP	Acceptance Data Package
ADP	Advanced Development Program
ADSF	Automated Directional Solidification Furnace
AEO	Assurance Engineering Office
AFD	Aft Flight Deck
AFEQ	Adiabatic Fast Equilibration
AFT	Advanced Furnace Technology
AIAA	American Institute of Aeronautics and Astronautics
ALF	Acoustic Levitator Furnace
ALU	Advanced Levitation Unit
AME	Acceleration Monitoring Experiment
AMO	Assurance Management Office
AO	Announcement of Opportunity
AOMS	Advanced Optical Monitoring Systems
APCF	Advanced Protein Crystallization Facility
APCG	Advanced Protein Crystal Growth
APCGF	Advanced Protein Crystal Growth Facility
APM	Attached Payload Module

AR	Acceptance Review
ARC	Aggregation of Red Blood Cells (Australia)
ARC	Ames Research Center
ARF	Animal Research Facility
ASCG	Automatic Solution Crystal Growth
ASCO	Specific Change Order
ASTP	Apollo-Soyuz Test Project
ATAC	Advanced Technology Advisory Committee
ATCS	Active Thermal Control Subsystem
ATD	Advanced Technology Development
ATE	Automatic Test Equipment
ATP	Authority to Proceed
AUE	Alloy Undercooling Experiment
AVCG	Automatic Vapor Crystal Growth
B/L	Baseline
BASE	Binary Alloy Solidification Experiment
BASG	Ball Aerospace Group
BBU	Bubble Behavior Unit (Japan)
BCL	Battelle Columbus Laboratories
BDPU	Bubble, Drop and Particle Unit
BF	Biotechnology Facility
BIO	Space Bioreactor
BiSn	Bismuth-Tin Crystal Growth
BIU	Bus Interface Unit
BRE	Blood Rheology Equipment
BTF	Biotechnology Facility
BTS	Biotelemetry System
C	Celsius
C&T	Communications and Tracking
C/C	Carrier/Container
C/O	Checkout
CAD	Computer-Aided Design
CADAP	Computer-Aided Dendrite Analysis Program
CAE	Computer-Aided Engineering
CAG	Commercial Advocacy Group
CAM	Computer-Aided Manufacturing
CAP	Crew Activity Plan
CAP	Customer Accommodation Plan
CAST	Casting and Solidification Technology

CBE	Chemical Beam Epitaxy
CCB	Change Control Board
CCB	Configuration Control Board
CCD	Charge-coupled Device
CCDS	Centers for the Commercial Development of Space
CCTV	Closed Circuit Television
CDG	Concept Development Group
CDMS	Command and Data Management System
CDOT	Colloidal Disorder-Order Transitions
CDR	Critical Design Review
CDSF	Commercially Developed Space Facility
CEI SPEC	Contract End Item Specification
CELS	Controlled Environment and Life Support System
CELSS	Controlled Environment and Life Support System
CER	Cost Estimate Relationships
CET	Combined Environmental Test
CF	Constant Flux
CFES	Continuous Flow Electrophoresis System
CFIF	Continuous Flow Isoelectric Focusing
CFLSE	Critical Fluid Light Scattering Experiment
CFM	Candle Flames in Microgravity
CFTE	Critical Fluid Thermal Equilibration Experiment
CFVME	Critical Fluid Viscosity Measurement Experiment
CGF	Crystal Growth Furnace
CHF	Continuous Heating Furnace (Japan)
CI	Customer Integration
CIO	Customer Integration Office
CIEF	Continuous Isoelectric Focusing
CIP	Customer Integration Panel
CITE	Cargo Integration Test Equipment
cm	Centimeter
CM-1	Combustion Module
CMDSF	Crystals, Monomers, Deposition and Separation Facility
CMG	Control Moment Gyro
CNES	Centre Nationale d'Études Spatiales
CO	Contracting Officer
CoDR	Conceptual Design Review
COMLAB	Commerce Lab
COMM	Commercial Missions

COS	Co-Orbiting Satellite
COTR	Contracting Officer Technical Representative
COTS	Commercial Off The Shelf
CPF	Critical Point Facility
CPL	Capillary Pumped Loop
CPSE	Common Payload Support Equipment
CRR	Cargo Readiness Review
CRT	Character Recognition Terminal
CRU	Catalytic Research Unit
CSA	Canadian Space Agency
CSC	Consulting Support Center
CSD	Comparative Soot Diagnostics
CSD	Contract Start Date
CSS-IPS	Common Support System-Integrated Payload System
CT	Constant Temperature
CTL	Communications Test Lab
CVD	Chemical Vapor Deposition
CVTE	Chemical Vapor Transport Experiment
CW	Continuous Wave
DACS	Digital Acquisition and Control System
DARA	Deutsche Agentur für Raumfahrtangelegenheiten [German Space Agency]
DARTFire	Diffusive and Radiative Transport in Fires
DAS	Data Acquisition System
DBMS	Data Base Management System
dc	Direct Current
DCDU	Digital Cassette Data Unit
DCE	Droplet Combustion Experiment
DCF	Droplet Combustion Facility
DCR	Design Certification Review
DCR	Drawing Change Request
DDF	Directors Discretionary Fund
DDM	Data Display Module
DDM	Drop Dynamics Module
DDS	Data Display System
DDT&E	Design, Develop, Test, and Evaluation
DDU	Data Display Unit
DEL	Delivery
DEP	Dedicated Experiment Processor
DFRC	Hugh L. Dryden Flight Research Center

DFVLR	Deutsche Forschungs-und Versuchsanstalt für Luft-und
DIF	Data Interchange Format
DLR	The German Aerospace Research Establishment
DMOS	Diffusive Mixing of Organic Solutions
DMS	Data Management System
DOC	Discipline Operations Center
DOD	Department of Defense
DOMSAT	Domestic Satellite
DPA	Data Processing Assembly
DPIMS	Diffusion Processes in Molten Semiconductors
DPM	Drop Physics Module
DPRO	Defense Procurement Resident Office
DR	Data Requirement
DSC	Differential Scanning Calorimetry
DSF	Directional Solidification Furnace
DT/DT	Drop Tube/Drop Tower (Facility)
DTA	Differential Thermal Analysis
DTA	Development Test Article
DTA	Differential Thermal Analysis
DTD	Droplet Technology Demonstration
DTF	Drop Tube/Tower Facility
DTO	Detailed Test Objective
DVT	Developmental Vibration Test
DWG	Discipline Working Group
EAC	Experiment Apparatus Container
EALK	External Airlock
EBF	Electron Bombardment Furnace
ECAS	Experiment Computer Applications Software
ECE	Experiment Checkout Equipment
ECG	Electroepitaxial Crystal Growth (MRA)
ECLSS	Environmental Control/Life Support System
ECOS	Experiment Computer Operational Software
ECP	Electromagnetic Containerless Processing
ECS	Energy Conversion Subsystem
ECS	Environmental Control Subsystem
ED	Engineering Directorate
EDEP	Electrodeposition (UAH)
EDM	Engineering Development Model
EDO	Extended Duration Orbiter

EDR	Engineering Design Review
EDS	Energy Dispersive Spectroscopy
EEE	Electronic, Electrical, Electromechanical
EEP	Experiment Electronic Package
EEVT	Electrophoresis Equipment Verification Test
EGSE	Electrical Ground Support Equipment
EHD	Electrohydrodynamic
EICG	Electronic/Infrared Crystal Growth
EIRD	Experiment Interface Requirements Document
ELV	Expendable Launch Vehicle
EM	Engineering Model
EMC	Electromagnetic Compatibility
EMDI	Extended Mission Duration Items
EMI	Electromagnetic Interference
EML	Electromagnetic Levitator
EMS	Engineering Master Schedule
EMS	Experiment Mounting Structure
EMU	Extravehicular Maneuvering Unit
EMU	Extravehicular Mobility Unit
EOM	Earth Observation Mission
EOM	Engineering Operations Manual
EOS	Earth Observing System
EOS	Electrophoresis Operations in Space (MDAC)
EPDP	Experiment Power Distribution Box
EPROM	Erasable Programmable Read-Only Memory
EPS	Electrical Power System
ERD	Experiment Requirements Document
ESA	European Space Agency
ESD	Electrostatic Discharge
ESE	Electrical Support Equipment
ESM	Experiment Service Module
ESPS	Experiment Segment/Pallet Simulator
ESRO	European Space Research Organization
ESS	Energy Storage Subsystem
ESS	Experiment Subsystem Simulator
ET	External Tank
ETE	External Test Equipment
EU	Electronics Unit
EURECA	European Retrievable Carrier

EVAS	Extravehicular Activity System
EXP	Experiment
FA	Flight Accommodation
FAR	Final Acceptance Review
FAWG	Flight Assignments Working Group
FCA	Flow Control Assembly
FDD	Flight Data Document
FDE	Fluid Dynamics Experiment
FDF	Flight Data File
FDOR	Final Design and Operations Review
FDR	Final Design Review
FDSMM	Fluid Dynamics and Solidification of Metallic Melts
FEA	Fluids Experiment Apparatus
FEP	Front End Processor
FES	Fluids Experiments System
FES	Flash Evaporator System (an Orbiter subsystem)
FES	Fluids Experiment System
FES/VCGS	Fluid Experiment/Vapor Crystal Growth System
FF	Free Flyer
FFDF	Fluid Physics and Dynamics Facility
FFEU	Free-Flow Electrophoresis Unit
FFFT	Forced Flow Flamespread Test
FHA	Flight Hardware Availability
FMEA-CIL	Failure Modes and Effects Analyses/Critical Items List
FMPT	First Material Processing Test (Japan)
FO	Functional Objectives
FOR	Flight Operations Review
FOV	Field of View
FPDF	Fluid Physics/Dynamics Facility
FPE	Fundamental Phenomena Experimentation
FRB	Failure Review Board
FRE	Functional Requirements Envelope
FRR	Flight Readiness Review
FS	Factor of Safety
FSD	Fabrication Support Division
FSDC	Fiber Supported Droplet Combustion
FSDM	Free Surface Deformation Measurement System
FSS	Flight Support System
FSUWG	Facility Science Users Working Group

FU	Flight Unit
FY	Fiscal Year
FZCGF	Float Zone Crystal Growth Facility (Battelle)
FZES	Float Zone Experiment System
g	Gravity
g ₀	normal gravity acceleration at sea-level
GaAs	Gallium Arsenide
GAC	Grumman Aerospace Corporation
GAS	Get-Away-Special
GAS Can	Get-away Special Canister
GAS Can	Get-Away-Special Canister
GBX	Glovebox
GC-MS	Gas Chromatograph-Mass Spectrometer
GCE	Ground Control Experiment
GCEL	Ground Control Experiment Laboratory
GDFE	Gas-Jet Diffusion Flames Experiment
GEF	Gas Evaporation Experiment Facility (Japan)
GEM	Generic Experiment Module
GEO	Geosynchronous Earth Orbit
GERME	Groupe D'Etude et Recherches, Sur Test Materieux Dans
GEVS	General Environmental Verification Specification
GFE	Government Furnished Equipment
GFFC	Geophysical Fluid Flow Cell
GFGAS	Gradient Furnace for Get Away Special
GFP	Glass Fiber Pulling
GFP	Government Furnished Property
GH	Growth Hormone
GHF	Gradient Heating Facility
GHF	Gradient Heating Furnace (Japan)
GIDEP	Government/Industry Data Exchange Program
GIFFTS	Gravitational Influences on Flammability and Flamespread
GIRD	Ground Integration Requirements Document
GMT	Greenwich Mean Time
GN&C	Guidance, Navigation and Control
GOR	Ground Operations Review
GPC	General Purpose Computer
GPF-1&2	General Purpose Furnace
GPRF-G	General Purpose Rocket Furnace-Gradient
GPRF-I	General Purpose Rocket Furnace -Isothermal

GPS	Global Position Satellite
GPS	Global Positioning System
GPU	Ground Power Unit
GSE	Ground Support Equipment
GSFC	Goddard Space Flight Center
GT	Ground Test
H/W	Hardware
HAB	Habitability
HAL	High-temperature Acoustic Levitator
HAL/S	High-Order Programming Language for Spacelab Usage
HDR	High Data Rate
HDRR	High Data Rate Recorder
HDW	Hardware
HGCS	Human Granulocyte Colony Stimulating
HGS	Holographic Ground System
HH-G	Hitchhiker (Goddard)
HH-M	Hitchhiker (MSFC)
HHVT	High Resolution, High Frame Rate Video Technology
HIA	Holographic Imaging Apparatus
HM	Habitation Module
HMF	Health Maintenance Facility
HOSC	Huntsville Operations Support Center
HPA	Handling and Positioning Aid
HPCG	Hand-held Protein Crystal Growth
HPF	Heat Pipe Furnace
HPIR	Heat Pipe Radiator
HQ	Headquarters
HRAP	Heat Rejection Augmentation Package
HRF	Human Research Facility
HRM	High Rate Multiplexer
HRT	High-Resolution Thermometer
HTFT	High Temperature Furnace Technology
HTGPF	High Temperature General Purpose Furnace
HTM	High Temperature Materials
HX	Heat Exchanger
Hz	Hertz (Cycles per Second)
IBSE	Initial Blood Storage Experiment
ICD	Interface Control Document
ICD	Interface Control Drawing

ICE	Interface Configuration Experiment
IDE	Initial Design Evaluation
IDGE	Isothermal Dendritic Growth Experiment
IDGE	Isothermal Dendrite Growth Experiment
IDMS	Information and Data Management System
IEF	Isoelectric Focusing Experiment
IF	Intermediate Frequency
IFF	Isoelectric Focusing Facility
IFM	Interface Measurements
IG	Igloo (Spacelab Pallet Missions)
IGI	Industrial Guest Investigator
IH/SR	Integration Hardware/Software Review
IHF	Isothermal (Japan)
II	Industrial Investigator
IIA	Instrument Interface Agreements
IM	Interface Measurements
IMF	Image Furnace (Japan)
IML	International Microgravity Laboratory
IMU	Inertial Measurement Unit
INEPT	EN Engineering Panel Telemail
IOC	Initial Operating Capability
IOC	Initial Orbiting Capability
IOU	Input/Output Unit
IPL	Integrated Payload
IPRD	Integrated Payload Requirements Document
IPS	Instrument Pointing System
IR&D	Independent Research and Development
IRD	Interface Requirements Document
IRIG	Inter-range instrumentation group (time format in Spacelab)
IRR	Initial Requirements Review
IRR	Integration Readiness Review
IRR	Interface Requirements Review
IRSM	Incubator Refrigerator Storage Module
ISA	Inertial Sensor Assemblies
ISC	International Space Corporation
ISSET	Intercenter Systems Engineering Team
ISF	Industrial Space Facility
ISR	Interim Systems Review
ISSP	Information System Strategic Plan

ISTF	Integrated Services and Test Facility (Canada)
ISY	International Space Year (1992)
ITA	Instrumentation Technology Associates, Inc.
ITIP	International Technology Integration Panel
ITUS	Integrated Thermal Utility System
IVA	Intravehicular Activity
IWG	Investigator Working Group
JCA	Joint Cooperative Agreement
JEA	Joint Endeavor Agreement
JEM	Japanese Experiment Module
JIS	Joint Integration Simulation
JPL	Jet Propulsion Laboratory
JSC	Johnson Space Center
JSLWG	Joint Spacelab Working Group
JURG	Joint User Requirements Group
K	Kelvin
KBPS	Kilobytes Per Second
kg	Kilogram
KSC	Kennedy Space Center
LAB	Laboratory
LAN	Local Area Network
LaRC	Langley Research Center
LASS	Large Amplitude Space Simulator
LBTF	Langmuir-Blodgett Trough Facility
LDEF	Long Duration Exposure Facility
LDF	Liquid Drop Experiment Facility (Japan)
LDR	Large Deployable Reflector
LDR	Low Data Rate
LDV	Laser Doppler Velocimetry
LDV	Laser Doppler Velocimetry
LED	Light Emitting Diode
LEO	Low Earth Orbit
LeRC	Lewis Research Center
LIF	Large Isothermal Furnace
LIMS	Lewis Information Management System
LLSI	Laser Light Scattering Instrument
LM	Logistics Module
LME	Liquid Motion Experiment
LMI	Lewis Management Instruction

LOS	Line of Sight
LOS	Loss of Signal
LPE	Lambda Point Experiment
LPES	Lamda Point Experiment System
LPS	Launch Processing System
LPS	Liquid Phase Sintering
LS	Life Sciences
LSA	Large Space Antenna
LSE	Laboratory Support Equipment
LSLAB	Life Sciences Laboratory
LSRF	Life Sciences Research Facility
LSSP	Launch Site Support Plan
LSW	Lifshitz, Slyozov and Wagner (Theory of Alloys)
LTE	Levitor Technology Experiment (ACES II)
LTGHE	Low-Temperature Gradient Heating Furnace
LTRF	Low Temperature Research Facility
LVLH	Local Vertical, Local Horizontal
LVLH	Local Vertical, Local Horizontal Meter
μg	Microgravity
m	Meter
M&P	Materials and Processes
MA	Mission Assignment
MA	Multiple Access
MAC	Microgravity Advisory Committee
MAP	Mission Activity Plan
MAS	Metals/Alloy Solidification
MASA	Metals and Alloys Solidification Apparatus
MASU	Metal Alloy Separation Unit
MAUS	Materialwissen Autonomoe Experi Uter Schwerelosigkeit
MBE	Molecular Beam Epitaxy
MBPS	Megabytes Per Second
MCC	Mission Control Center
MCD	Modular Capabilities Document
MCDS	Management Communications and Data System
MCF	Modular Combustion Facility
MCP	Monitoring Control Panel
MCPF	Modular Containerless Processing Facility
MCU	Marangoni Convection Unit
MD	Middeck

MDAC	MacDonnell Douglas Aerospace Corporation
MDB	Master Data Base
MDE	Mission Dependent Equipment
MDM	Multiplexer/Demultiplexer
MDTSCO	MacDonnell Douglas Technical Services Company
MEA	Materials Experiment Assembly
MEL	Modular Electromagnetic Levitator
MEM	Middeck Electronics Module
MEPF	Multiple Experiment Processing Furnace
MEPHISTO	Matériel pour l'Étude des Phénomènes Intéressants
MFCD	Microgravity Fluids and Combustion Diagnostics
MFCT	Modular Furnace Component Technology
MGM	Mechanics of Granular Materials
MGSE	Mechanical Ground Support Equipment
MHF	Mirror Furnace (ESA)
MHRR	MSAD Hardware Reflight Review
MIA	Mission Implementation Agreement
MIC	Management Information Center
MICG	Mercury Iodide Crystal Growth
MICOM	Mission Command
MINC	Module Interconnect
MIP	Mission Integration Panel
MIS	Magnetic Isolation System
MIS	Management Information System
MIT	Massachusetts Institute of Technology
MIUL	Material Identification and Usage List
MLI	Multilayer Insulation
MLR	Monodisperse Latex Reactor
MLRS	Monodisperse Latex Reactor System
MLSA	Modified Launch Services Agreement
MMAP	Microgravity Measurement and Analysis Project
MMFF	Modular Multizone Furnace Facility (now SSFF)
MMO	Mission Management Office Meeting
MMP	Magnetospheric Multiprobe
MMPF	Microgravity and Materials Processing Facility
MMSL	Microgravity Materials Science Laboratory
MMU	Manned Maneuvering Unit
MMU	Mass Memory Unit
MOD	Module

MORD	Mission Operations Requirements Document
MOU	Memorandum of Understanding
MP	Microgravity Pressure
MP	Major Payload
MPA	Microgravity Pressure, Ambient
MPAK	Middeck Payload Accommodation Kit
MPE	Mission Peculiar Equipment
MPES	Mission Peculiar Experiment Support Structure
MPS	Materials Processing in Space
MRA	Mechanical Readiness Assessment
MRA	Microgravity Research Associates
MRB	Material Review Board
MRD	Mission Requirements Document
MRDB	Mission Requirements Data Base
MRI	Midwest Research Institute
MRMS	Mobile Remote Manipulator System
MROFIE	Mission Requirements on Facilities/Instruments/Experiments
MRR	Mission Readiness Review
MRWG	Mission Requirements Working Group
MS	Margin of Safety
MS	Materials Science
MSA	Microgravity Science and Applications (Program)
MSAD	Microgravity Science and Applications Division
MSC	Microgravity Smoldering Combustion Experiment
MSDR	Materials Science Double Rack
MSEIS	Microgravity Systems Engineering Information System
MSFC	Marshall Space Flight Center
MSL	Microgravity Science Laboratory
MST	Measurement Status Table
MTE	Mass Transport Experiment
MTL	Manufacturing and Technology Laboratory
MTPE	Mission to Planet Earth (NASA)-Code Y
MTU	Master Timing Unit
MUA	Material Utilization Agreement
MWEU	Moving Wall Electrophoresis Unit
MWSF	Molecular Wake Shield Facility
NAC	NASA Advisory Council
NAR	Non-Advocate Review
NASA	National Aeronautics and Space Administration

NASACOM	NASA Communications System
NASDA	National Space Development Agency of Japan
NBS	National Bureau of Standards
NCC	NASA Communications Control
NCTM	Non-Contact Temperature Measurements
NFF	Normal Freezing Furnace
NHB	NASA Handbook
NIA	Network Interface Adapter
NIH	National Institutes of Health
NIST	National Institute for Standards and Technology
NIU	Network Interface Unit
NLO	Nonlinear Optical
NLOMTF	Non-Linear Optical Monomer Thin Films (UAH)
NLOOC	Non-Linear Optical Organic Crystals (UAH)
nm	Nanometers
nm	Nautical Miles
NMI	NASA Management Instruction
NMMSA	NASA Microgravity Materials Science Assessment Task Force
NOA	New Obligation Authority
NOAA	National Oceanic and Atmospheric Administration
NRA	NASA Research Announcement
NRC	National Research Council
NRL	Naval Research Laboratory
NSF	National Science Foundation
NSPAR	Nonstandard Parts Approval Request
NSSDC	National Space Science Data Center
NSTL	National Space Technology Laboratories
NSTS	National Space Transportation System
O&C	Operations and Checkout
OACT	Office of Advanced Concepts and Technology
OAFD	Orbiter Aft Flight Deck
OARE	Orbital Acceleration Research Experiment
OCF	Organic Crystal Growth Facility (ESA)
OCP	Office of Commercial Programs (NASA) - Code I
OCZ	Operational Control Zone
OFFPU	Optical Fiber Production Unit
OFT	Orbital Flight Test
OIA	Orbiter Interface Adaptor
OLMSA	Office of Life Sciences and Microgravity Applications

OMCVD	Organometallic Chemical Vapor Epitaxy
OMRS	Operations and Maintenance Requirements Specifications
OMS	Orbital Maneuvering System
OMS&A	Office of Mission Safety and Assurance
OMU	Orbital Maneuvering Unit
OMV	Orbital Maneuvering Vehicle
OPCGA	Observable Protein Crystal Growth Apparatus
OPCGF	Organic and Polymer Crystal Growth Facility
OPF	Orbiter Processing Facility
OPPE	Organic and Polymer Processing Experiment (3M)
ORAM	Orbital Repair and Maintenance
ORSEP	Organic Separation
ORU	Orbital Replacement Unit
OSF	Office of Space Flight (NASA) - Code M
OSO	Office of Space Operations (NASA) -Code T
OSS	Office of Space Science (NASA) - Code S
OSS	Office of Space Station (NASA) - Code S
OSTDS	Office of Space Tracking and Data Systems (NASA) - Code T
OSV	Orbital Servicing Vehicle (Japan)
OSV	Orbiting Servicing Vehicle (Japan)
OTA	Office of Technology Assessment
OTFE	Oscillatory Thermocapillary Flow Experiment
OTV	Orbital Transfer Vehicle
PA	Power Amplifier
PA	Product Assurance
PACE	Physics and Chemistry Experiment Program
PACS	Pointing And Control System
PAD	Program Approval Document
PaDR	Payload Design Review
PAI	Product Assurance Instruction
PAM	Payload Accommodation Manager
PAM	Payload Assist Module
PAM	Project Assurance Manager
PAM	Project Assurance Manual
PAP	Product Assurance Plan
PBE	Pool Boiling Experiment
PC	Personal Computer
PCA	Payload Clamp Assembly
PCB	Power Control Box

PCCE	Particle Cloud Combustion Experiment
PCDA	Power Control and Distribution Assembly
PCG	Protein Crystal Growth
PCGS	Protein Crystal Growth System
PCM	Pulse Code Modulation
PCM	Pulse Code Modulator
PCR	Payload Certification Review
PCTC	Payload Crew Training Complex
PCU	Payload Checkout Unit
PCU	Power Control Unit
PCU	Power Conversion Unit
PDA	Phase Doppler Pneumometer
PDI	Particle Displacement Interferometry
PDP	Plasma Diagnostics Package
PDR	Preliminary Design Review
PDRD	Program Definition and Requirements Document
PDSS	Payload Development Support System
PE	Principle Engineer
PED	Payload Element Developer
PEPWG	Pressurized Element Working Group
PF	Platform
PFA	Post-Flight Annex
PFDAR	Post-Flight Data Analysis Review
PFM	Protoflight Model
PFM	Program and Financial Plan
PGS	Power Generation Subsystem
pH	Hydrogen Ions in Gram Atoms per Liter
PI	Payload Interrogator
PI	Preliminary Investigation
PI	Principal Investigator
PIC	Project Initiation Conference
PID	Prime Item Development (Spec)
PID	Program Introduction Document
PID	Proportional, Integral, and Differential Gain
PIMS	Principal Investigator Microgravity Services
PIP	Payload Integration Plan
PIV	Particle Image Velocimetry
PL	Payload
PM	Program Manager

PM	Project Manager
PMAD	Power Management and Distribution
PMC	Permanent Manned Capability
PMIC	Payload Missions Integration Contractor
PMMS	Process Material Management System
PMR	Program Management Review
PMT	photomultiplier tube
PMZF	Programmable Multizone Furnace
POCC	Payload Operations Control Center (at MSFC)
POD	Payload Operations Director
POIC	Payload Operation and Integration Center
POO	Pallet of Opportunity
POOC	Payload of Opportunity Carrier
POP	Perpendicular to Orbit Plane
POP	Program Operating Plan
POWG	Payload Operations Working Group
PP	Phase Partitioning
PP	Planning Package
PP&C	Payload Planning and Control
PP/L	Partial Payload
PPE	Phase Partitioning Experiment
PPO	Planning Purposes Only
PRACA	Problem Reporting and Corrective Action
PRCB	Program Requirements Change Board
PRE	Performance Requirements Envelope
PROM	Programmable Read-Only Memory
PRR	Preliminary Requirements Review
PRR	Program Requirements Review
PS	Payload Specialist
PS	Phase Separation
PS	Project Scientist
PSC	Performing Support Center
PSCN	Program Support Communications Network
psia	Pounds Per Square Inch Absolute
PSR	Pre-Ship Review
PV	Photovoltaic
PVT	Physical Vapor Transport
PVTOS	Physical Vapor Transport of Organic Solutions (3M)
QA	Quality Assurance

QE	Quality Engineering
QSAM	Quasi-steady Acceleraton Measurement System
R&D	Research and Development
R&M	Reliability and Maintainability
R&PM	Research and Program Management
RAHF	Research Animal Holding Facility
RAPIV	Radiographic Particle Image Velocimetry
RAU	Remote Acquisition Unit
RBFS	Risk-Based Fire Safety
RCB	Requirements Change Board
RCG	Reference Concept Group
RCS	Reaction Control System
RDR	Requirements Definition Review
RDR	Requirements Definition Review
RF	Radio Frequency
RFI	Radio Frequency Interference
RFP	Request For Proposal
RFQ	Request For Quotation
RI	Rockwell International
RID	Review Item Discrepancy
RIEF	Recirculating Isoelectric Focusing
RITSI	Radiative Ignition and Transition to Spread Investigation
RKT	Rocket
RMMR	Reactionless Microgravity Mechanisms and Robotics
RMS	Remote Manipulator System
ROC	Regional Operations Center
RP	Reference Publication
RP	Rocket Propellant
RPCVD	Remote Plasma-enhanced Chemical Vapor Epitaxy
RPDP	Recoverable Plasma Diagnostics Package
RPI	Rensselaer Polytechnic Institute
RR	Requirements Review
RSD	Rainbow Schlieren Deflectometry
RTE	Radiative Transfer Equation
RTOP	Research and Technology Operations Plans
RTS	Remote Triaxial Sensors
RUR	Reference Update Review
RUR	Requirements Update Review
S&T	Science and Technology (Center)

S&TWG	Science and Technology Working Group
S/L	Spacelab
S/W	Software
SAA	South Atlantic Anomaly
SAA	Science And Applications
SAAC	Space Applications Advisory Committee
SAAG	Science and Applications Advocacy Group
SAAL	Single-Axis Acoustic Levitator
SAAR	Small and Rapid Response
SAAX	Science and Applications Missions (No.)
SAB	Space Applications Board
SAGE	Standard Assurance Guidelines for Experiments
SAIL	Shuttle Avionics Integration Laboratory
SAL	Spread Across Liquids
SAMPIE	Solar Array Module Plasma Interaction Experiment
SAMS	Space Acceleration Measurement Systems
SAMS-FF	Space Acceleration Measurement System for Free Flyers
SAMS-II	Space Acceleration Measurement System for International Space Station
SAO	Safety Assurance Office
SATS	Station Accommodation Test Sets
SBIR	Small Business Innovative Research
SCD	Source Control Document
SCEF	Stress Corrosion Evaluation Form
SCES	Static Column Electrophoretic Separator
SCF	Supercritical Fluid
SCG	Solution Crystal Growth
SCIF	Static Column Isoelectric Focusing
SCO	Schedule Coordinating Office
SCOS	Subsystem Computer Operating System
SCU	Signal Control Unit
SCU	System Control Unit
SDA	Solute Diffusion Apparatus
SDR	System Design Review
SDT	Science Definition Team
SE&I	System Engineering and Integration
SEB	Source Evaluation Board
SED	Space Experiments Division
SEDCCS	SED Configuration Control System
SEF	Space Experiment Facility

SEID	Spacelab Experiment Interface Device
SEL	Space Experiments Laboratory
SEM	Scanning Electron Microscopy
SEMS	Shuttle Environment Monitoring System
SEP	Support Electronics Package
SESAC	Space and Earth Science Advisory Committee
SESCO	Severe Environment Systems Company
SHAP	Sample Handling and Analysis Plan
SI	International System of Units
SIB	System Integration Board
SII	Space Industries, Inc.
SIM	Simulation
SIMS	Simulations of Spacelab Missions
SIPS	Spacelab Input Processing System
SIR	Systems Integration Review
SIV	Stereo Imaging Velocimeter
SL	ESA Spacelab (in Space Shuttle cargo bay; e.g., IML and USML)
SL-D1	First German Spacelab
SL-D2	Second German Spacelab
SL-J	Japanese Spacelab
SLDPF	Spacelab Data Processing Facility
SLS	Spacelab Life Sciences
SLS	Spacelab Simulator
SLSI	Surface Light Scattering Instruments
SM	Short Module
SOPS	Spacelab Output Processing System
SOTA	State of The Art
SOW	Statement Of Work
SPA	Small Payload Accommodations
SPA	Software Product Assurance
SPAH	Spacelab Payload Accommodation Handbook
SPAR	Space Processing Applications Rocket
SPAR	Standard Payload Assurance Requirements
SPAS	German Shuttle Pallet Satellite
SPGEN	Space Station Planning Group, EN
SPICE	Spacelab Payload Integration and Coordination in Europe
SPL	Sonic Pump Levitator
SPPO	Spacelab Payload Project Office (MSFC)
SPS	Samples Per Second

SPSME	Spacelab Payload Standard Modular Electronics
SQUID	Superconducting Quantum Interference Detector
SR	Science Requirements
SR&QA	Safety, Reliability, and Quality Assurance
SRB	Solid Rocket Booster
SRD	Science Requirements Document
SRD	Shuttle Requirements Definition
SRD	Shuttle Requirements Document
SRD	Software Requirements Document
SRR	Site Readiness Review
SRR	System Requirements Review
SS	Space Station
SSB	Space Science Board
SSC	Support Service Contractor
SSCB	Space Station Control Board
SSCC	Space Station Control Center
SSCE	Solid Surface Combustion Experiment
SSDMS	Space Station Data Management System
SSDS	Space Station Data Systems
SSFF	Space Station Furnace Facility
SSIP	Shuttle Student Involvement Project
SSIS	Space Station Information System
SSOTF	Space Station Operations Task Force
SSP	Space Station Program
SSPE	Space Station Program Element
SSSAAS	Space Station Science and Applications Advisory Subcommittee
SSSC	Space Station Support Center
SSST	Space Station Systems Trainer
SSWP	Space Station Work Package
STAMPS	Scientific and Technological Aspects of Materials Processing
STB	Science and Technology Board
STD	Standard
STDCE	Surface Tension Driven Convection Experiment
STEF	Space Test and Evaluation Facility
STEP	Satellite Test of the Equivalence Principle
STEP	Space Technology Experiments Platform
STR	System Test Review
STS	Space Transportation System
STS	Shuttle Transportation System

STS	Space Transportation System
STT	Spacelab Transfer Tunnel
SURF	Space Ultra-vacuum Research Facility
SVP	Space Vehicle Pressure
SW	Software
T&C	Telemetry And Command
T/L	Timeline
TAG	Technology Advocacy Group
TBD	To Be Determined
TBD	To Be Done
TBE	Teledyne Brown Engineering
TBS	Thermal Bus System
TC	Thermal Control
TCR	Technical and Cost Review
TCS	Test Control Supervisor
TCS	Test Control System
TCS	Thermal Control Subsystem
TCS	Thermal Control System
TDAS	Tracking and Data Acquisition Satellite
TDASS	Tracking and Data Acquisition Satellite System
TDL	Technology Development Laboratory
TDM	Technology Development Missions
TDMP	Technology Development Missions Polar (Canada)
TDMX	Technology Development Missions (No.)
TDP	Technology Development Program
TDRS	Tracking and Data Relay Satellite
TDRSS	Tracking and Data Relay Satellite System
TEA	Technical Exchange Agreement
TEA	Torque Equilibrium Attitude
TEM	Transmission Electron Microscopy
TEMPUS	Electromagnetic Containerless Processing Facility
TEQb	Thermal Equilibration-bis
TES	Thermal Energy Storage
TEZG	Tribological Experiments in Zero Gravity
TFCG	Thin Film Crystal Growth
TFDU	Thin Film Deposition Unit
TFSUS	Task Force on Scientific Uses of the Space Station
TGDF	Turbulent Gasjet Diffusion Flames
TGDF	Transitional/Turbulent Gas Jet Diffusion Flames

TGS	Telemetry Ground Station
TGS	Telemetry Ground System
TGS	Triglycine Sulfate
THR	Test Hardware Received
TID	Test Installation Division
TIM	Technical Interchange Meeting
TLM	Telemetry
TME	Test and Measurement Equipment
TMIS	Technical and Management Information System
TMM	Thermal Mathematical Model
TMS	Thermal Maneuvering System
TPC	Technical Performance Criteria
TPCE	Tank Pressure Control Experiment
TPFE	Two-Phase Flow Experiment
TRW	Thompson Ramo Woolridge
TSS	Tethered Satellite System
TT&C	Telemetry, Tracking and Command
TU	Technology Utilization
TU	Transport Unit
U.S.	United States
U.S.C.	United States Code
U/D	Update
UAB	University of Alabama in Birmingham
UAH	University of Alabama in Huntsville
UCSD	University of California, San Diego
UIO	User Integration Office
UISWG	User Information System Working Group
UMRIS	User Mission Requirements and Information System
UOF	User Operation Facility
UPN	Unique Project Number
USAF	United State Air Force
USL	United States Laboratory
USML	United States Microgravity Laboratory
USML-2	United States Microgravity Laboratory-2
USMP	United States Microgravity Payload
USMP-2	United States Microgravity Payload-2
USRA	Universities Space Research Association
UTC	User Time Clock
V	Volts

VAB	Vehicle Assembly Building
VAFB	Vandenberg Air Force Base
VAK	Vertical Access Kit
VCAP	Vehicle Charging and Potential
VCG	Vapor Crystal Growth
VCGS	Vapor Crystal Growth System
VDA	Vapor Diffusion Apparatus
VDC	Volts Direct Current
VER	Verification
VET	Video Event Trigger
VFI	Verification Flight Instrumentation
VHSIC	Very High Speed Integrated Circuit
VIBES	Vibration Isolation in a Box Experiment System
VIT	Vibration Isolation Technology
VITR	Video/Instrumentation Tape Recorder
VMA	Vacuum Maintenance Assembly
VPF	Vertical Processing Facility
VTRE	Vented Tank Resupply Experiment
WBR	Workbench Rack
WBRIS	Workbench Rack Illuminations Subassembly
WBS	Work Breakdown Structure
WCS	Waste Control System
WFF	Wallops Flight Facility
WIF	Wire Insulation Flammability Experiment
WP	Work Package
WSGT	White Sands Ground Terminal
WTR	Western Test Range
WWV	National "Time Standard" Call Letters
XRD	X-ray Diffraction
ZCG	Zeolite Crystal Growth
ZENO	Critical Fluid Scattering Experiment (CFLSE)
ZOE	Zone of Exclusion

S. Aibara — Kyoto University (Japan)

W. F. Anderson — Northwestern University Medical School

E. Arnold — Rutgers University

Y. S. Babu — BioCryst Pharmaceuticals, Inc.

J. K. Baird — University of Alabama, Huntsville

J. Bertrand — Institut de Biologie Structurale (France)

C. Betzel — AG Makromolekulare Strukturanalyse (Germany)

D. Carter — NASA Marshall Space Flight Center (MSFC)

C. W. Carter, Jr. — University of North Carolina, Chapel Hill

D. Chattopadhyay — University of Alabama at Birmingham

E. W. Czerwinski — University of Texas, Medical Branch

L. T. Delbaere — University of Saskatchewan (Canada)

L. J. DeLucas — University of Alabama, Birmingham

J. Drenth — University of Groningen (The Netherlands)

D. J. Duchamp — The Upjohn Company

D. S. Eggleston — Smith Kline Beecham Pharmaceuticals

H. M. Einspahr — Bristol-Meyers Squibb

O. El-Kabbani — University of Alabama at Birmingham

G. K. Farber — Pennsylvania State University

B. C. Finzel — The Upjohn Company

J. Fontecilla Camps — I.B.S. - L.C.C.P. (France)

R. A. Grant — Atlantic BioPharmaceuticals, Inc.

P. L. Howell — Hospital for Sick Children (Canada)

N. D. Jones — Eli Lilly Research

J. R. Knox — University of Connecticut

K. L. Krause — University of Houston

W. G. Laver — The Australian National University (Australia)

P. Lu — University of Pennsylvania

M. Luo — University of Alabama at Birmingham

A. McPherson — University of California, Riverside

E. J. Meehan — University of Alabama, Huntsville

E. F. Meyer — Texas A&M University

T. L. Nagabhushan — Schering-Plough Research Institute

R. J. Naumann — University of Alabama, Huntsville

D. H. Ohlendorf — University of Minnesota

S. Quirk — Georgia Institute of Technology

P. Reichert — Schering-Plow Research Institute

P. G. Righetti — University di Milano (Italy)

F. R. Salemme — 3-Dimensional Pharmaceuticals, Inc.

V. K. Senadhi — Temple University

J. Sevcik — Slovak Academy of Sciences (Slovak Republic)

L. Sieker — University of Washington

P. B. Sigler — Yale University

R. J. Sirko — McDonnell Douglas Aerospace

G. D. Smith — Medical Foundation of Buffalo

R. S. Snyder — NASA Marshall Space Flight Center (MSFC)

M. D. Spangfort — ALK A/S (Denmark)

N. Sthanam — University of Alabama at Huntsville

M. Sundaralingam — Ohio State University

R. M. Sweet — Associated Universities, Inc.

F. P. Tally — Cubist Pharmaceuticals, Inc.

J. Thomson — Vertex Pharmaceuticals, Inc.

D. Voet — University of Pennsylvania

M. Walter — University of Alabama at Birmingham

B. Wang — University of Georgia

K. Ward — Naval Research Laboratory (NRL)

K. D. Watenpugh — The Upjohn Company

P. C. Weber — Schering-Plough Research Institute

W. Weber — University of Hamburg (Germany)

L. D. Williams — Georgia Institute of Technology

W. W. Wilson — Mississippi State University

D. Yang — McMaster University (Canada)

A. Yonath — DESY/MPG (Germany)

Dr. Reza Abbaschian	Department of Materials Science and Engineering University of Florida 132 Rhines Hall Gainesville, FL 32611-2066	Office Ph: 904 392-1454 Fax: 904 392-6359	137
Dr. Davood Abdollahian	S. Levy Incorporated 3425 South Bascom Avenue Campbell, CA 95008	Office Ph: 408 369-3865 Fax: 408 371-6804	454, 456
Prof. Bruce J. Ackerson	Department of Physics Oklahoma State University Stillwater, OK 74078	Office Ph: 405 744-5796 Fax: 405 744-6811	457
Prof. Ajay K. Agrawal	School of Aerospace and Mechanical Engineering University of Oklahoma 865 Asp Avenue, Room 212 Norman, OK 73019	Office Ph: 405 325-1754 Fax: 405 325-1088	346
Prof. Guenter Ahlers	Director, Center for Nonlinear Sciences Quantum Institute University of California, Santa Barbara Santa Barbara, CA 93106	Office Ph: 805 893-3795 Fax: 805 893-4170	706, 708
Prof. J. Iwan D. Alexander	Center for Microgravity and Materials Research University of Alabama, Huntsville Huntsville, AL 35899	Office Ph: 205 890-6887 Fax: 205 890-6791	459, 460, 770
Dr. Spiro D. Alexandratos	Department of Chemistry University of Tennessee, Knoxville 575 Buehler Hall Knoxville, TN 37996-1600	Office Ph: 423 974-3399 Fax: 423 974-3454	772
Mr. A. P. Allan	University of Delaware 1200 Sycamore Street Wilmington, DE 19805	Office Ph: 302 575-1991	992
Dr. M. C. Altan	School of Aerospace and Mechanical Engineering University of Oklahoma Norman, OK 73019	Office Ph: 405 325-1737 Fax: 405 325-1088	774

Prof. Robert A. Altenkirch	Dean, College of Engineering and Architecture Washington State University 146 Dana Hall Pullman, WA 99164-2714	Office Ph: 509 335-5593 Fax: 509 335-9608	25, 27, 29
Prof. C. D. Andereck	Department of Physics Ohio State University 174 West 18th Avenue Columbia, OH 43210	Office Ph: 614 292-2360 Fax: 614 292-7557	462
Prof. John L. Anderson	Dean, College of Engineering Carnegie Mellon University Pittsburgh, PA 15213-3890	Office Ph: 412 268-2537 Fax: 412 268-6421	465
Dr. Timothy J. Anderson	Department of Chemical Engineering University of Florida 227 Chemical Engineering Building Gainesville, FL 32611	Office Ph: 352 392-0882 Fax: 352 392-9513	777, 778
Dr. J. B. Andrews	Department of Materials & Mechanical Engineering BEC 360 University of Alabama, Birmingham 1150 Tenth Avenue South Birmingham, AL 35294-4461	Office Ph: 205 934-8452 Fax: 205 934-8485	139, 780
Prof. Robert E. Apfel	Robert Higgin Professor of Mechanical Engineering Department of Mechanical Engineering Yale University 9 Hillhouse Avenue, Room M-1, P.O. Box 208286 New Haven, CT 06520-8286	Office Ph: 203 432-4346 Fax: 203 432-7654	75, 782
Dr. Alan J. Ardell	Department of Materials Science and Engineering 6531-G BH University of California, Los Angeles 405 Hilgard Avenue Los Angeles, CA 90095-1595	Office Ph: 310 825-7011 Fax: 310 206-7353	784
Prof. Stephen Arnold	Department of Applied Math and Physics Polytechnic University Six Metrotech Center Brooklyn, NY 11201	Office Ph: 718 260-3085 Fax: 718 260-3139	786

Prof. Arvind Atreya	Department of Mechanical Engineering and Applied Mechanics College of Engineering University of Michigan 2158 G. G. Brown Building Ann Arbor, MI 48109-2125 Office Ph: 313 747-4790 Fax: 313 747-3170	348
Prof. C. T. Avedisian	Sibley School of Mechanical and Aerospace Engineering Cornell University Ithaca, NY 14853-7501 Office Ph: 607 255-5105 Fax: 607 255-1222	350, 467
Prof. Richard L. Axelbaum	Department of Mechanical Engineering Campus Box 1185 Washington University One Brookings Drive St. Louis, MO 63130 Office Ph: 314 935-7560 Fax: 314 935-4014	352
Prof. Portonovo S. Ayyaswamy	Department of Mechanical Engineering & Applied Mechanics School of Engineering and Applied Science University of Pennsylvania Philadelphia, PA 19104-6315 Office Ph: 215 898-8362 Fax: 215 573-6334	197
Dr. William D. Bachalo	President Aerometrics, Inc. 755 North Mary Avenue Sunnyvale, CA 94086 Office Ph: 408 738-6688 Fax: 408 738-6871	354
Dr. Klaus J. Bachmann	Department of Materials Science and Engineering Campus Box 7919 North Carolina State University Raleigh, NC 27695-7919 Office Ph: 919 515-2538 Fax: 919 515-3419	142
Dr. M. Y. Bahadori	Power and Information Systems Division Science Applications International Corporation 21151 Western Avenue Torrance, CA 90501-1724 Office Ph: 310 781-8723 Fax: 310 781-8730	31
Prof. Vemuri Balakotaiah	Department of Chemical Engineering University of Houston Houston, TX 77204-4792 Office Ph: 713 743-4318 Fax: 713 743-4323	77
Prof. Sanjoy Banerjee	Department of Chemical Engineering University of California, Santa Barbara Santa Barbara, CA 93106 Office Ph: 805- 893-3456 Fax: 805 893-4731	469

Prof. S. G. Bankoff	Department of Chemical Engineering Northwestern University 2145 Sheridan Road Evanston, IL 60208	Office Ph: 847 491-5267 Fax: 847 491-3728	470
Dr. Martin B. Barmatz	Technical Group Leader Mail Stop 183-401 Jet Propulsion Laboratory (JPL) California Institute of Technology 4800 Oak Grove Drive Pasadena, CA 91109-8099	Office Ph: 818 354-3088 Fax: 818 393-5039	127, 710
Dr. Mark A. Barteau	Department of Chemical Engineering University of Delaware Newark, DE 19716	Office Ph: 302 831-8905 Fax: 302 831-2085	788
Dr. Osman A. Basaran	School of Chemical Engineering 1283 Chemical Engineering Bldg. Purdue University West Lafayette, IN 47907-1283	Office Ph: 317 494-4061 Fax: 317 494-0805	472
Dr. James C. Baygents	Department of Chemical and Environmental Engineering University of Arizona Harshbarger Building, Room 120 Tucson, AZ 85721	Office Ph: 520 621-6044 Fax: 520 621-6048	474
Dr. Robert J. Bayuzick	Department of Applied and Engineering Science Vanderbilt University 610 Olin Hall Nashville, TN 37240	Office Ph: 615 322-7047 Fax: 615 343-8645	144, 147, 790
Jeanne L. Becker, Ph.D.	Department of Obstetrics and Gynecology University of South Florida 4 Columbia Drive Tampa, FL 33606	Office Ph: 813 254-7774 Fax: 813 254-0940	200
Prof. Christoph Beckermann	Department of Mechanical Engineering University of Iowa Iowa City, IA 52242	Office Ph: 319 335-5681 Fax: 319 335-5669	149, 793, 795
Prof. Robert P. Behringer	Department of Physics Duke University Box 90305 Durham, NC 27708-0305	Office Ph: 919 660-2550 Fax: 919 660-2525	476

Dr. Robert F. Berg	Thermophysics Division National Institute of Standards and Technology Building 221, Room A111 Gaithersburg, MD 20899	Office Ph: 301 975-2466 Fax: 301 869-4020	79
Prof. Luis P. Bernal	Department of Aerospace Engineering University of Michigan 1320 Beal Avenue Ann Arbor, MI 48109-2118	Office Ph: 313 764-3396 Fax: 313 763-0578	477
Prof. Rajendra S. Bhatnagar	Laboratory of Connective Tissue Biochemistry University of California, San Francisco Box 0424, S0512 San Francisco, CA 94143-0424	Office Ph: 415 476-2923 Fax: 415 476-4204	203
Dr. Lynn A. Boatner	Head, Ceramics and Interfaces Section Solid State Division Mail Stop 6056 Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831	Office Ph: 423 574-5492 Fax: 423 574-4814	797
Dr. Stephen T. Boyd	Department of Physics and Astronomy University of New Mexico 800 Yale Boulevard, P.O. Box 5800 Albuquerque, NM 87131-1156	Office Ph: 505 277-4439 Fax: 505 277-1520	712
Dr. Jeremiah U. Brackbill	Theoretical Division Los Alamos National Laboratory T-3, Fluid Dynamics, B216 Los Alamos, NM 87545	Office Ph: 505 667-8811 Fax: 505 665-5926	478
Dr. John F. Brady	Division of Chemistry and Chemical Engineering California Institute of Technology Pasadena, CA 91125	Office Ph: 818 395-4183 Fax: 818 568-8743	799
Prof. Melvyn C. Branch	Department of Mechanical Engineering Campus Box 427 University of Colorado, Boulder Engineering Center Boulder, CO 80309-0427	Office Ph: 303 492- 6318 Fax: 303 492-2863	356

Dr. Kenneth Brezinsky	Department of Chemical Engineering University of Illinois at Chicago 810 South Clinton Street Chicago, IL 60607-7000	Office Ph: 312-996-9430	800
Dr. Robert A. Brown	Dean, School of Engineering Massachusetts Institute of Technology Building 1, Room 206 77 Massachusetts Avenue Cambridge, MA 02139-4307	Office Ph: 617 253-5726 Fax: 617 253-8549	802, 804, 806
Prof. John D. Buckmaster	University of Illinois at Urbana-Champaign Room 321 Talbot Lab 104 Wright Street Urbana, IL 61801	Office Ph: 217 333-1803 Fax: 217 244-0720	358
Dr. Kathryn M. Butler	Materials Fire Research Group Mail Stop B258 National Institute of Standards & Technology Building and Fire Research Laboratory Building 224 Gaithersburg, MD 20899	Office Ph: 301 975-6673 Fax: 301 975-4052	362
Prof. Van P. Carey	Department of Mechanical Engineering University of California, Berkeley 6185 Etcheverry Hall Berkeley, CA 94720	Office Ph: 510 642-7177 Fax: 510 642-6163	480
Dr. Charles W. Carter	Department of Biochemistry and Biophysics University of North Carolina, Chapel Hill Campus Box 7260 Chapel Hill, NC 27599-7260	Office Ph: 919 966-3263 Fax: 919 966-2852	205
Dr. Daniel C. Carter	Chief, Biophysics Branch Microgravity Science and Applications Division Mail Code ES76 NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812	Office Ph: 205 544-5492 Fax: 205 544-1777	9, 1031
Prof. Peggy Cebe	Department of Physics and Astronomy Tufts University Science & Technology Center, Room 208 4 Colby Street Medford, MA 02155	Office Ph: 617 627-3365 Fax: 617 627-3744	808

Prof. David M. Ceperley	Department of Physics University of Illinois, Urbana-Champaign 1110 West Green Street Urbana, IL 61801	Office Ph: 217 244-0646 Fax: 217 244-2909	713
Dr. Ared Cezairliyan	Metallurgy Division Materials Science and Engineering Laboratory National Institute of Standards and Technology Building 236 Gaithersburg, MD 20899	Office Ph: 301 975-5931 Fax: 301 990-2572	810, 812
Dr. Soyoung S. Cha	Department of Mechanical Engineering 2039 ERF University of Illinois at Chicago 842 West Taylor Street Chicago, IL 60607-7022	Office Ph: 312 996-9612 Fax: 312 413-0447	813
Dr. An-Ti Chai	Mail Stop 500-102 NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191	Office Ph: 216 433-2073 Fax: 216 433-8050	482, 484
Prof. Paul M. Chaikin	Department of Physics Princeton University P.O. Box 708 Princeton, NJ 08544	Office Ph: 609 258-4338 Fax: 609 258-6360	81
Prof. S. H. Chan	Department of Mechanical Engineering University of Wisconsin, Milwaukee P.O. Box 784 Milwaukee, WI 53201	Office Ph: 414 229-5001 Fax: 414 229-6958	486
Dr. Robert G. Chave	Science and Technology Development Section Section 354 Mail Stop 79-24 Jet Propulsion Laboratory (JPL) 4800 Oak Grove Drive Pasadena, CA 91109-8099	Office Ph: 818 393-2556 Fax: 818 393-4878	994
Prof. H. K. Chelliah	Department of Mechanical, Aerospace, and Nuclear Engineering School of Engineering & Applied Science University of Virginia Thornton Hall Charlottesville, VA 22903-2442	Office Ph: 804 924-6037 Fax: 804 982-2037	364

Prof. Chuan F. Chen	Department of Aerospace and Mechanical Engineering College of Engineering & Mines University of Arizona Tucson, AZ 85721	Office Ph: 520 621-8199 Fax: 520 621-8191	488
Prof. L.- D. Chen	Department of Mechanical Engineering The University of Iowa Iowa City, IA 52242	Office Ph: 319 335-5674 Fax: 319 335-5669	365
Dr. Robert K. Cheng	Combustion Group Energy & Environment Division Lawrence Berkeley Laboratory 1 Cyclotron Road Berkeley, CA 94720	Office Ph: 510 486-5438 Fax: 510 486-7303	369
Prof. Norman Chigier	Department of Mechanical Engineering Carnegie Mellon University Schenley Park Pittsburgh, PA 15213-3890	Office Ph: 412 268-2498 Fax: 412 268-3348	490
Prof. Mun Y. Choi	Department of Mechanical Engineering Mail Code 251 University of Illinois, Chicago 842 West Taylor Street Chicago, IL 60607-7022	Office Ph: 312 996-7389 Fax: 312 413-0447	34
Dr. Talso C. Chui	Mail Stop 79-24 Jet Propulsion Laboratory (JPL) California Institute of Technology 4800 Oak Grove Drive Pasadena, CA 91109-8099	Office Ph: 818 354-3104 Fax: 818 393-4878	714, 715, 716
Prof. Jacob N. Chung	Department of Mechanical and Materials Engineering Washington State University Pullman, WA 99164-2920	Office Ph: 509 335-3222 Fax: 509 335-4662	492
Prof. Leland W. Chung	Urology Research Laboratory Department of Urology Box 422 University of Virginia Health Sciences Center Charlottesville, VA 22908	Office Ph: 804 243-6649 Fax: 804 243-6648	207

Dr. Ivan O. Clark	Information & Electromagnetic Technology Division Mail Stop 473 NASA Langley Research Center 8 North Dryden Street Hampton, VA 23681-0001 Office Ph: 757 864-1500 Fax: 757 864-7891	495, 815
Prof. Noel A. Clark	Department of Physics University of Colorado, Boulder Campus Box 390 Boulder, CO 80309-0390 Office Ph: 303 492-6420 Fax: 303 492-2998	497, 499
Prof. Paul Concus	Lawrence Berkeley Laboratory Mail Stop 50A-2129 University of California, Berkeley 1 Cyclotron Road Berkeley, CA 94720 Office Ph: 510 486-5508 Fax: 510 486-5401	501, 504
Dr. Reid F. Cooper	Department of Materials Science and Engineering University of Wisconsin 1509 University Avenue Madison, WI 53706 Office Ph: 608 262-1133 Fax: 608 262-8353	817
Dr. Sam R. Coriell	Metallurgy Division National Institute of Standards and Technology A153 Materials Building Gaithersburg, MD 20899 Office Ph: 301 975-6169 Fax: 301 975-2128	505
Dr. Gerard L. Cote	Bioengineering Program Texas A&M University 233 Zachry Engineering Center College Station, TX 77843-3120 Office Ph: 409 845-4196 Fax: 409 847-9005	210
Dr. Peter A. Curreri	Crystal Growth & Solidification Branch Microgravity Science & Applications Division Mail Code ES75 NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812 Office Ph: 205 544-7763 Fax: 205 544-6660	819, 996
Prof. Arnold Dahm	Physics Department Case Western Reserve University 10900 Euclid Avenue Cleveland, OH 44106 Office Ph: 216 368-3586 Fax: 216 368-4671	821

Dr. Jonathan A. Dantzig	Department of Mechanical and Industrial Engineering Mail Code 244 University of Illinois at Urbana-Champaign 138 Mechanical Engineering Building 1206 West Green Street Urbana, IL 61801	Office Ph: 217 333-4107 Fax: 217 244-6534	823
Dr. E. J. Davis	Department of Chemical Engineering Mail Stop BF-10 University of Washington Seattle, WA 98195	Office Ph: 206 543-2250 Fax: 206 543-3778	507
Prof. Robert H. Davis	Department of Chemical Engineering University of Colorado, Boulder Campus Box 424 Boulder, CO 80309-0424	Office Ph: 303 492-7314 Fax: 303 492-4341	509, 511, 513
Prof. Stephen H. Davis	Department of Engineering Sciences and Applied Mathematics Northwestern University 2145 Sheridan Road Evanston, IL 60208	Office Ph: 847 491-5397 Fax: 847 491-2178	515, 517
Dr. Lawrence J. DeLucas	Center for Macromolecular Crystallography 79-THT, BHSB 262 University of Alabama at Birmingham 1918 University Boulevard Birmingham, AL 35294-0005	Office Ph: 205 934-5329 Fax: 205 934-0480	11, 214, 216
Dr. Jeffrey J. Derby	Department of Chemical Engineering and Materials Science 151 Amundson Hall University of Minnesota 421 Washington Avenue S.E. Minneapolis, MN 55455-0132	Office Ph: 612 625-8881 Fax: 612 626-7246	825
Dr. George T. DeTitta	Hauptman-Woodward Medical Research Institute 73 High Street Buffalo, NY 14203-1196	Office Ph: 716 856-9600 Fax: 716 852-4846	218
Dr. Vijay K. Dhir	Engineering Department University of California, Los Angeles Los Angeles, CA 90024	Office Ph: 310 825-8507 Fax: 310 206-4830	83

Dr. Daniel L. Dietrich	Mail Stop 110-3 NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191	Office Ph: 216 433-8759 Fax: 216 433-3793	38, 370
Dr. S. D. Dimitrijevic	Health Science Center at Fort Worth University of North Texas 3500 Camp Bowie Boulevard Fort Worth, TX 76107-2699	Office Ph: 817 735-2125 Fax: 817 735-2133	220
Dr. Ellen R. Dirksen	Department of Neurobiology UCLA School of Medicine 73-235 CHS University of California, Los Angeles Box 951763 Los Angeles, CA 90095-1763	Office Ph: 310 825-9565 Fax: 310 825-2224	223
Prof. Russell J. Donnelly	Department of Physics University of Oregon Eugene, OR 97403-1274	Office Ph: 541 346-4226 Fax: 541 346-4708	717, 718
Dr. Edward L. Dreizin	AeroChem Research Laboratories, Inc. P.O. Box 12 Princeton, NJ 08542-0012	Office Ph: 609 716-1201 Fax: 609 716-1201	372, 374
Prof. James F. Driscoll	University of Michigan 3004 FXB Building Ann Arbor, MI 48109-2118	Office Ph: 313 936-0101 Fax: 313 763-0578	376
Dr. Michael Dudley	Department of Materials Science and Engineering State University of New York, Stony Brook Stony Brook, NY 11794-2275	Office Ph: 516 632-8500 Fax: 516 632-8052	827, 830
Prof. Robert V. Duncan	Department of Physics and Astronomy University of New Mexico 800 Yale Street Albuquerque, NM 87131-1156	Office Ph: 505 277-4507 Fax: 505 255-1520	128
Prof. Douglas J. Durian	Department of Physics University of California, Los Angeles 405 Hilgard Avenue Los Angeles, CA 90024	Office Ph: 310 206-2645 Fax: 310 825-0897	86, 518

Dr. Don J. Durzan	Department of Environmental Horticulture University of California, Davis Davis, CA 94616-8587	Office Ph: 916 752-0399 Fax: 916 752-0399	227
Prof. Prabir K. Dutta	Department of Chemistry Ohio State University 120 West 18th Avenue Columbus, OH 43210	Office Ph: 614 292-4532 Fax: 614 292-1685	834, 836
Dr. Pierre Echternach	Mail Stop 79-24 Jet Propulsion Laboratory (JPL) California Institute of Technology 4800 Oak Grove Drive Pasadena, CA 91109-8099	Office Ph: 818 393-3563 Fax: 818 393-4878	998
Prof. Boyd F. Edwards	Department of Physics West Virginia University P.O. Box 6315 Morgantown, WV 26506-6315	Office Ph: 304 293-3422 Fax: 304 293-5732	520
Prof. Fokion N. Egolfopoulos	Department of Mechanical Engineering University of Southern California Olin Hall 430 Los Angeles, CA 90089-1453	Office Ph: 213 740-0480 Fax: 213 740-8071	379, 381
Dr. M. S. El-Shall	Department of Chemistry Virginia Commonwealth University Richmond, VA 23284-2006	Office Ph: 804 828-3518 Fax: 804 828-8599	837
Prof. Charles Elbaum	Department of Physics Brown University Box 1843 Providence, RI 02912	Office Ph: 401 863-2186 Fax: 401 863-2024	719, 721
Prof. Said E. Elghobashi	Department of Mechanical & Aerospace Engineering University of California, Irvine Irvine, CA 92717	Office Ph: 714 824-6131 Fax: 714 824-8585	382, 522
Prof. C. W. F. Everitt	Hansen Experimental Physics Laboratory Gravity Probe B Stanford University Stanford, CA 94305-4085	Office Ph: 415 725-4103 Fax: 415 725-8312	130

Prof. Gerard M. Faeth	Department of Aerospace Engineering College of Engineering University of Michigan 1320 Beal Avenue Ann Arbor, MI 48109-2118	Office Ph: 313 764-7202 Fax: 313 936-0106	40, 384
Prof. Amir Faghri	Department of Mechanical Engineering School of Engineering University of Connecticut 191 Auditorium Road Storrs, CT 06226	Office Ph: 203 486-0419 Fax: 203 486-5088	524
Dr. Alexandre I. Fedoseyev	Center for Microgravity and Materials Research University of Alabama, Huntsville Huntsville, AL 35899	Office Ph: 205 890-6889 Fax: 205 890-6791	839
Dr. Robert S. Feigelson	Center for Materials Research Stanford University Stanford, CA 94305	Office Ph: 415 723-4007 Fax: 415 723-3044	230
Dr. Frank Fendell	TRW Space & Technology Division TRW Space and Electronics Group One Space Park Redondo Beach, CA 90278	Office Ph: 310 812-0327 Fax: 310 812-7589	44
Prof. A. C. Fernandez-Pello	Department of Mechanical Engineering University of California, Berkeley Etcheverry Hall Berkeley, CA 94720	Office Ph: 510 642-6554 Fax: 510 642-6163	47, 53
Prof. Richard A. Ferrell	Department of Physics and Astronomy University of Maryland, College Park College Park, MD 20742	Office Ph: 301 405-6148 Fax: 301 314-9465	88, 723
Dr. Merton C. Flemings	Department of Materials Science & Engineering Massachusetts Institute of Technology Room 8-407 77 Massachusetts Avenue Cambridge, MA 02139-4307	Office Ph: 617 253-3233 Fax: 617 258-6886	150, 151, 841
Prof. John A. Frangos	Department of Bioengineering University of California, San Diego 9500 Gilman Drive La Jolla, CA 92093	Office Ph: 619 534-0421 Fax: 619 534-5722	232

Mr. David J. Frank	O/92-10, B/205 Lockheed Martin Missiles & Space Company 3251 Hanover Street Palo Alto, CA 94304-1187	Office Ph: 415 354-5311 Fax: 415 354-5415	726
Dr. Donald O. Frazier	Space Sciences Laboratory Mail Code ES01 NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812	Office Ph: 205 544-7825 Fax: 205 544-2102	843
Lisa E. Freed, M.D., Ph.D.	Division of Health Sciences & Technology Mail Code E25-342 Massachusetts Institute of Technology 77 Massachusetts Avenue Cambridge, MA 02139-4307	Office Ph: 617 253-3858 Fax: 617 258-8827	235, 237
Dr. Archibald L. Fripp	Sensors Research Branch Information and Electromagnetic Technology Division Mail Stop 473 NASA Langley Research Center 5 North Dryden Street Hampton, VA 23681	Office Ph: 757 864-1503 Fax: 757 864-7891	153, 845
Dr. D. T. Gallagher	Center for Advanced Research in Biotechnology 9600 Gudelsky Drive Rockville, MD 20850	Office Ph: 301 975-5726 Fax: 301 330-3447	243
Prof. Robert W. Gammon	Institute for Physical Science and Technology University of Maryland, College Park Building 85 College Park, MD 20742	Office Ph: 301 405 4791 Fax: 301 314-9509	132
Prof. Stephen Garoff	Department of Physics Carnegie Mellon University Pittsburgh, PA 15213-3890	Office Ph: 412 268-6877 Fax: 412 681-0648	90
Prof. Alice P. Gast	Department of Chemical Engineering Stanford University Stanford, CA 94305-5025	Office Ph: 415 725-3145 Fax: 415 725-7294	525, 527
Prof. Randall M. German	Department of Engineering Science Pennsylvania State University 118 Research West University Park, PA 16802-1401	Office Ph: 814 863-8025 Fax: 814 863-8211	155

Prof. Kurt Gibble	Sloane Physics Laboratory Yale University 12 Prospect Place, P. O. Box 208120 New Haven, CT 06511-8120 Office Ph: 203 432-6365 Fax: 203 432-7138	728
Dr. Donald C. Gillies	Crystal Growth & Solidification Branch Microgravity Science and Applications Division Mail Code ES75 NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812 Office Ph: 205 544-9302 Fax: 205 544-8762	847, 1000
Mr. Thomas K. Glasgow	Mail Stop 105-1 NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191 Office Ph: 216 433-5014 Fax: 216 433-5033	849
Prof. Martin E. Glicksman	Materials Engineering Department MRC-104 Rensselaer Polytechnic Institute Troy, NY 12180-3590 Office Ph: 518 276-6721 Fax: 518 276-8554	159
Dr. Joe D. Goddard	Department of Applied Mechanics and Engineering Sciences 0411 University of California, San Diego 9500 Gilman Drive La Jolla, CA 92093-0411 Office Ph: 619 534-4508 Fax: 619 534-4543	529
Prof. Arun M. Gokhale	School of Materials Science and Engineering Georgia Institute of Technology 778 Atlantic Drive Atlanta, GA 30332-0245 Office Ph: 404 894-2887 Fax: 404 894-9140	850, 852
Prof. Alessandro Gomez	Department of Mechanical Engineering Yale University New Haven, CT 06520 Office Ph: 203 432-4384 Fax: 203 432-7654	386
Steve R. Gonda, Ph.D.	Biotechnology Program Mail Code SD3 NASA Johnson Space Center 2101 NASA Road One Houston, TX 77058 Office Ph: 713 483-8745 Fax: 713 483-6227	244, 1002

Mr. Thomas J. Goodwin, M.S.	Biotechnology Program Mail Code SD3 NASA Johnson Space Center 2101 NASA Road One Houston, TX 77058	Office Ph: 713 483-7129 Fax: 713 483-3058	246
Dr. Ashok Gopinath	Department of Mechanical Engineering Code ME/Gk Naval Postgraduate School 700 Dyer Road, Room 333 Monterey, CA 93943-5108	Office Ph: 408 656-3400 Fax: 408 656-2238	530
Dr. John A. Goree	Department of Physics and Astronomy University of Iowa Iowa City, IA 52242-1479	Office Ph: 319 335-1843 Fax: 319 335-1753	854
Mr. Paul S. Greenberg	Mail Stop 110-3 NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191	Office Ph: 216 433-3621 Fax: 216 433-3793	1004
Prof. James B. Grotberg	Biomedical Engineering Department McCormick School of Engineering and Applied Science Northwestern University Evanston, IL 60208-3112	Office Ph: 847 491-3009 Fax: 847 491 4928	531, 534
Dr. Richard N. Grugel	Mail Stop ES75 Universities Space Research Association NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812	Office Ph: 205 544-9165 Fax: 205 544-8762	856, 858
Prof. Prabhat K. Gupta	Department of Materials Science and Engineering Ohio State University 2041 College Road Columbus, OH 43210	Office Ph: 614 292-6769 Fax: 614 292-1537	859
Prof. Hossein Haj-Hariri	Department of Mechanical, Aerospace, and Nuclear Engineering University of Virginia Thornton Hall Charlottesville, VA 22903-2037	Office Ph: 804 924-6290 Fax: 804 982-2037	536, 537

Prof. J. Woods Halley	Physics Department University of Minnesota 116 Church, SE Minneapolis, MN 55455	Office Ph: 612 624-0395 Fax: 612 624-4578	729
Prof. Kevin P. Hallinan	Department of Mechanical and Aerospace Engineering University of Dayton 300 College Park Dayton, OH 45469	Office Ph: 513 229-2875 Fax: 513 229-2756	538, 540
Dr. Timothy G. Hammond	Department of Internal Medicine Section of Neurology Mail Code SL45 Tulane University Medical Center 1430 Tulane Avenue New Orleans, LA 70112-2699	Office Ph: 504 588-5346 Fax: 504 584-1909	249
Dr. John E. Hart	Department of Astrophysics, Planetary, and Atmospheric Sciences Campus Box 391 University of Colorado at Boulder Boulder, CO 80309-0391	Office Ph: 303 492-8568 Fax: 303 492-3822	92
Dr. Charles R. Hartzell	Director of Research Alfred I. DuPont Institute of the Nemours Foundation P.O. Box 269 Wilmington, DE 19899	Office Ph: 302 651-6800 Fax: 302 651-6897	251
Prof. T. A. Hatton	Chevron Professor of Engineering Department of Chemical Engineering Massachusetts Institute of Technology 77 Massachusetts Avenue Cambridge, MA 02139-4307	Office Ph: 617 253-4588 Fax: 617 253-8723	541
Prof. Carole A. Heath	Department of Chemical Engineering Iowa State University 2114 Sweeney Hall Ames, IA 50011-2230	Office Ph: 515 294-4828 Fax: 515 294-2689	255
Dr. Uday Hegde	Mail Stop 500-115 NYMA, Inc. NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135	Office Ph: 216 433-8744 Fax: 216 433-8660	389

Dr. John Hegseth	Department of Physics University of New Orleans New Orleans, LA 70148	
	Office Ph: 504 286-6706 Fax: 504 286-6048	94, 543, 545
Dr. Daniel J. Heinzen	Department of Physics College of Natural Sciences University of Texas, Austin Austin, TX 78712	
	Office Ph: 512 471-3960 Fax: 512 471-9637	732, 734
Dr. Cila Herman	Department of Chemical Engineering G.W.C. Whiting School of Engineering Johns Hopkins University 3400 North Charles Street Baltimore, MD 21218-2694	
	Office Ph: 410 516-4467 Fax: 410 516-7254	546
Prof. Jean R. Hertzberg	Department of Mechanical Engineering Campus Box 427 University of Colorado, Boulder Boulder, CO 80309-0427	
	Office Ph: 303 492-5092 Fax: 303 492-2863	390
Dr. William H. Hofmeister	Department of Applied and Engineering Sciences Vanderbilt University 610 Olin Hall Nashville, TN 37240	
	Office Ph: 615 322-7053 Fax: 615 343-8645	860
Dr. Douglas E. Holmes	Telcom Devices Electronic Materials Engineering 829 Flynn Road Camarillo, CA 93012	
	Office Ph: 805 445-4500 Fax: 805 445-4502	862
Dr. R G. Holt	Department of Aerospace & Mechanical Engineering Boston University 110 Cummington Street Boston, MA 02215	
	Office Ph: 617 353-9594 Fax: 617 353-5866	548
Prof. George M. Homsy	Department of Chemical Engineering Stanford University Stanford, CA 94305	
	Office Ph: 415 723-2419 Fax: 415 723-9780	550, 552
Prof. Jack B. Howard	Department of Chemical Engineering Mail Code 66-454 Massachusetts Institute of Technology 77 Massachusetts Avenue Cambridge, MA 02139-4307	
	Office Ph: 617 253-4574 Fax: 617 258-5042	392

John H. Hughes, Ph.D.	Children's Hospital Ohio State University 308 Wexner 700 Children's Drive Columbus, OH 43205	Office Ph: 614 722-2795 Fax: 614 722-2716	257
Prof. Randall G. Hulet	Department of Physics Rice University P.O. Box 1892 Houston, TX 77251	Office Ph: 713 527-6087 Fax: 713 285-5492	736
Dr. Wesley C. Hymer	Department of Biochemistry and Molecular Biology Center for Cell Research Pennsylvania State University 206 South Frear Building University Park, PA 16802-6005	Office Ph: 814 865-2407 Fax: 814 865-2413	13
Dr. Marylou Ingram	Huntington Medical Research Institute 99 North El Molino Avenue Pasadena, CA 91101-1830	Office Ph: 818 795-4343 Fax: 818 795-5774	260
Dr. Ulf E. Israelsson	Mail Stop 79-3 Jet Propulsion Laboratory (JPL) California Institute of Technology 4800 Oak Grove Drive Pasadena, CA 91109-8099	Office Ph: 818 354-9255 Fax: 818 393-6383	737, 739, 1013
Dr. Kenneth A. Jackson	Department of Materials Science and Engineering Arizona Materials Laboratory University of Arizona 4715 East Fort Lowell Road Tucson, AZ 85712	Office Ph: 520 322-2981 Fax: 520 322-2993	864
Prof. Donald T. Jacobs	Physics Department The College of Wooster Wooster, OH 44691	Office Ph: 330 263-2390 Fax: 330 263-2516	553
Dr. Jeffrey W. Jacobs	Department of Aerospace and Mechanical Engineering University of Arizona Aero Building 16 Tucson, AZ 85721	Office Ph: 520 621-8459 Fax: 520 621-8191	95

Prof. David Jasnow	Department of Physics and Astronomy University of Pittsburgh Pittsburgh, PA 15260	Office Ph: 412 624-9029 Fax: 412 624-9163	554
Prof. James T. Jenkins	Department of Theoretical and Applied Mathematics Cornell University 212 Kimball Hall Ithaca, NY 14853	Office Ph: 607 255-7185 Fax: 617 255-2011	96
Dr. J. M. Jessup	Department of Surgery New England Deaconess Hospital Harvard Medical School 110 Francis Street, Suite 3A Boston, MA 02215	Office Ph: 617 632-9817 Fax: 617 632-7424	15, 263
Dr. Philip Johnson, M.D.	Department of Internal Medicine Room 1.122 MSB University of Texas Medical School at Houston 6431 Fannin Street Houston, TX 77030	Office Ph: 713 792-8347 Fax: 713 794-1734	265
Dr. William L. Johnson	Department of Materials Science Mail Code 138-78 California Institute of Technology Pasadena, CA 91125	Office Ph: 818 395-4433 Fax: 818 795-6132	163, 165
Dr. Monica L. Kafeory	Department of Materials Science and Engineering 330 White Building Case Western Reserve University 10900 Euclid Avenue Cleveland, OH 44106	Office Ph: 216 368-4219 Fax: 216 368-3209	866
Dr. K. Kailasanath	Laboratory for Computational Physics and Fluid Dynamics NRL Code 6410 Naval Research Laboratory Washington, DC 20375	Office Ph: 292 767-2402 Fax: 202 767-4798	393
Prof. Eric W. Kaler	Department of Chemical Engineering Colburn Laboratory University of Delaware Newark, DE 19716	Office Ph: 302 831-3553 Fax: 302 831-4466	556, 558

Dr. Yasuhiro Kamotani	Department of Mechanical and Aerospace Engineering Case Western Reserve University Cleveland, OH 44106	
	Office Ph: 216 368-6455 Fax: 216 368-6445	559
Dr. Daniel J. Kane	Southwest Sciences, Inc. 1570 Pacheco Street, Suite E-11 Santa Fe, NM 87505	
	Office Ph: 505 984-1322 Fax: 505 988-9230	395
Dr. Alain S. Karma	Department of Physics Northeastern University 111 Dana Research Center 360 Huntington Avenue Boston, MA 02115	
	Office Ph: 617 373-2929 Fax: 617 373-2943	867
Dr. Mark A. Kasevich	Department of Physics Stanford University Stanford, CA 94305	
	Office Ph: 415 725-1311 Fax: 415 723-9173	741
Dr. Takashi Kashiwagi	Center for Fire Research Building and Fire Research Laboratories National Institute of Standards and Technology Building 224, Room B258 Gaithersburg, MD 20899	
	Office Ph: 301 975-6699 Fax: 301 975-4052	55
Dr. Mohammad Kassemi	Mail Stop 105-1 Ohio AeroSpace Institute NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191	
	Office Ph: 216 433-5031 Fax: 216 433-5033	99, 560, 869, 871
Dr. Joseph L. Katz	Department of Chemical Engineering Johns Hopkins University 116 Maryland Hall Baltimore, MD 21218	
	Office Ph: 410 516-8484 Fax: 410 516-6463	873
Prof. Michael J. Kaufman	Department of Materials Science and Engineering University of Florida 201 Rhines Hall Gainesville, FL 32611-2066	
	Office Ph: 352 392-6662 Fax: 352 846-0403	875

Prof. Robert E. Kelly	School of Engineering and Applied Science 48-121 Engineering IV University of California, Los Angeles 408 Hilgard Avenue Los Angeles, CA 90024-1597	Office Ph: 310 825-5489 Fax: 310 206-4830	562, 564
Dr. Kenneth F. Kelton	Department of Physics Washington University at St. Louis Campus Box 1105 One Brookings Drive St. Louis, MO 63130	Office Ph: 314 935-6228 Fax: 314 935-6219	877
Prof. Edward G. Keshock	Mechanical Engineering Department Cleveland State University 1983 East 24th Street Cleveland, OH 44115	Office Ph: 216 687-2494 Fax: 216 687-9280	565
Prof. Jungho Kim	Department of Engineering University of Denver 2390 South York Street Denver, CO 80208	Office Ph: 303 871-3816 Fax: 303 871-4450	567, 568
Dr. Daniel A. Kirschner	Department of Biology Higgins Hall Boston College Chestnut Hill, MA 02167	Office Ph: 617 552-0211 Fax: 617 552-2011	268
Dr. John H. Konnert	Laboratory for the Structure of Matter Mail Code 6030 Naval Research Laboratory 4555 Overlook Avenue, SW Washington, DC 20375-6000	Office Ph: 202 767-3267 Fax: 202 767-6874	271
Prof. Joel Koplik	Department of Physics, Levich Institute City College of the City University of New York Convent Avenue and 138th Street New York, NY 10031	Office Ph: 212 650-8162 Fax: 212 650-6835	569, 571
Prof. Jean N. Koster	Department of Aerospace Engineering Sciences Campus Box 429 University of Colorado, Boulder Engineering Center Boulder, CO 80309-0429	Office Ph: 303 492-6945 Fax: 303 492-7881	101

Prof. Sindo Kou	Department of Materials Science and Engineering University of Wisconsin 1509 University Avenue Madison, WI 53706	Office Ph: 608 262-0576 Fax: 608 262-8353	573, 574
Dr. William B. Krantz	Department of Chemical Engineering Campus Box 424 University of Colorado at Boulder Engineering Center, ECCH 111 Boulder, CO 80309-0424	Office Ph: 303 492-7050 Fax: 303 492-4341	881
Dr. William E. Kraus	Department of Medicine Division of Cardiology Duke University Medical Center P.O. Box 3227 Durham, NC 27710	Office Ph: 919 684-3644 Fax: 919 684-8907	273
Dr. Anantha Krishnan	CFD Research Corporation 3325 Triana Boulevard Huntsville, AL 35805	Office Ph: 205 536-6576 Fax: 205 536-6590	883
Dr. Shankar Krishnan	Containerless Research, Inc. 910 University Place Evanston, IL 60261-3149	Office Ph: 708 467-2678 Fax: 708 467-2679	885
Prof. Jerry C. Ku	Mechanical Engineering Department Wayne State University 5050 Anthony Wayne Drive Detroit, MI 48202	Office Ph: 313 577-3814 Fax: 313 577-3881	396
Prof. Douglas A. Kurtze	Department of Physics North Dakota State University SU Station, Box 5566 Fargo, ND 58105-5566	Office Ph: 701 231-7048 Fax: 701 231-7088	887
Dr. Robert E. Kusner	Mail Stop 500-102 NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191	Office Ph: 216 433-9413 Fax: 216 433-3739	575
Prof. Richard T. Lahey	Nuclear Engineering and Engineering Physics Center for Multiphase Research Rensselaer Polytechnic Institute Troy, NY 12180-3590	Office Ph: 518 276-8579 Fax: 518 276-3055	577

Dr. Melora E. Larson	Mail Stop 79-24 Jet Propulsion Laboratory (JPL) California Institute of Technology 4800 Oak Grove Drive Pasadena, CA 91109-8099	Office Ph: 818 354-8751 Fax: 818 393-4878	744, 745
Prof. David J. Larson, Jr.	Materials Science and Engineering Engineering 318 State University of New York, Stony Brook Stony Brook, NY 11794-2275	Office Ph: 516 632-8485 Fax: 516 632-8052	167, 169
Prof. Chung K. Law	Department of Mechanical and Aerospace Engineering Princeton University Engineering Quadrangle Princeton, NJ 08544	Office Ph: 609 258-5271 Fax: 609 258-6233	398
Dr. L. G. Leal	Department of Chemical Engineering University of California, Santa Barbara Santa Barbara, CA 93106-5080	Office Ph: 805 893-8510 Fax: 805 893-7518	578
Dr. Sandor L. Lehoczký	Chief, Microgravity Science and Applications Division Mail Code ES71 NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812	Office Ph: 205 544-7758 Fax: 205 544-8762	171, 173
Dr. David T. Leighton	Department of Chemical Engineering University of Notre Dame Notre Dame, IN 46556	Office Ph: 219 631-6698 Fax: 219 631-8366	579
Dr. Peter I. Lelkes	Laboratory of Cell Biology Sinai Samaritan Medical Center University of Wisconsin Medical School Box 342 945 North 12th Street Milwaukee, WI 53201-0342	Office Ph: 414 219-7753 Fax: 414 219-7874	275
Prof. Elliot M. Levine	The Wistar Institute 3601 Spruce Street Philadelphia, PA 19104-4268	Office Ph: 215 898-3884 Fax: 215 898-0847	278
Dr. Ben Q. Li	Department of Mechanical Engineering Louisiana State University Baton Rouge, LA 70803	Office Ph: 504 388-6488 Fax: 504 388-5924	888

Prof. A. Liakopoulos	Department of Mechanical Engineering Lehigh University Bethlehem, PA 18015-3085	
	Office Ph: 610 758-4929 Fax: 610 758-6224	581
Prof. Seth Lichter	Department of Mechanical Engineering Northwestern University 2145 Sheridan Road Evanston, IL 60208-3111	
	Office Ph: 847 491-7470 Fax: 847 491-3915	583
Prof. Sung P. Lin	Department of Mechanical and Aeronautical Engineering Box 5725 Clarkson University Old Main Potsdam, NY 13699-5725	
	Office Ph: 315 268-6584 Fax: 315 268-6438	584, 586
Dr. Gregory T. Linteris	National Institute of Standards and Technology Building 224, Room B356 Gaithersburg, MD 20899	
	Office Ph: 301 975-2283 Fax: 301 975-4062	400
Prof. John A. Lipa	Department of Physics Stanford University Stanford, CA 94305-4060	
	Office Ph: 415 723-4562 Fax: 415 723-5584	134, 136, 746, 747, 748
Prof. Jing Liu	Department of Physics California State University, Long Beach 1250 Bellflower Boulevard Long Beach, CA 90840	
	Office Ph: 310 985-4913 Fax: 310 985-7924	103, 588
Dr. Bruce R. Locke	Department of Chemical Engineering FAMU/FSU College of Engineering Florida State University 2525 Pottsdamer Street Tallahassee, FL 32310-6046	
	Office Ph: 904 487-6165 Fax: 904 487-6150	282
Prof. Michael Loewenberg	Department of Chemical Engineering Mason Laboratory Yale University 9 Hillhouse Avenue New Haven, CT 06520	
	Office Ph: 203 432-4334 Fax: 203 432-7232	590
Dr. Thomas A. Lograsso	Institute for Physical Research and Technology Iowa State University 111 Metals Development Building Ames, IA 50011	
	Office Ph: 515 294-8425 Fax: 515 294-8727	890

Prof. Marshall B. Long	Department of Mechanical Engineering Yale University P.O. Box 208284 New Haven, CT 06520	Office Ph: 203 432-4229 Fax: 203 432-6775	403
Dr. Daniel W. Mackowski	Department of Mechanical Engineering Auburn University 201 Ross Hall Auburn, AL 36849-5341	Office Ph: 334 844-3334 Fax: 334 844-3307	591, 892
Prof. James V. Maher	Department of Physics and Astronomy University of Pittsburgh Pittsburgh, PA 15260	Office Ph: 412 624-4223 Fax: 412 383-9640	592
Prof. Charles Maldarelli	Levich Institute & Department of Chemical Engineering The City College of CUNY Covent Avenue at 138th Street New York, NY 10031	Office Ph: 212 650-8160 Fax: 212 650 -6835	594
Dr. Alexander J. Malkin	Department of Biochemistry University of California, Riverside 900 University Avenue Riverside, CA 92521	Office Ph: 909 787-3397 Fax: 909 787-3790	283
Prof. Efstratios Manousakis	Department of Physics Florida State University 318 Keen Building, B-159 Tallahassee, FL 32306-3016	Office Ph: 904 644-3713 Fax: 904 644-8630	749, 751
Dr. Stephen B. Margolis	Combustion Research Facility Department 8351 Mail Stop 9051 Sandia National Laboratories Livermore, CA 94551-0969	Office Ph: 510 294-3073 Fax: 510 294-1004	404
Prof. Humphrey J. Maris	Physics Department Brown University Providence, RI 02912	Office Ph: 401 863-2185 Fax: 401 863-2024	753
Prof. Philip L. Marston	Department of Physics Washington State University Pullman, WA 99164-2814	Office Ph: 509 335-5343 Fax: 509 335-7816	597, 599

Andreas Martin, M.D.	Division of Endocrinology/Metabolism Department of Medicine Mount Sinai Medical Center Mount Sinai School of Medicine 1 Gustave L. Levy Place New York, NY 10029-6574	Office Ph: 212 241-9528 Fax: 212 241-4218	286
Mr. Larry W. Mason	Payloads, Sensors, & Instruments Mail Stop B0560 Lockheed Martin Astronautics P.O. Box 179 Denver, CO 80201	Office Ph: 303 971-9067 Fax: 303 977-0829	17
Prof. Moshe Matalon	McCormick School of Engineering Northwestern University 2145 Sheridan Road Evanston, IL 60208-3125	Office Ph: 847 491-5396 Fax: 847 491-2178	405
Dr. Lon J. Mathias	Department of Polymer Science University of Southern Mississippi Southern Station Box 10076 Hattiesburg, MS 39406-0076	Office Ph: 601 266-4871 Fax: 601 266-5504	894
Prof. Bernard J. Matkowsky	Department of Engineering Sciences of Applied Mathematics Northwestern University Evanston, IL 60208	Office Ph: 847 491-5397 Fax: 847 491-2178	408
Prof. David H. Matthiesen	Department of Materials Science and Engineering Case Western Reserve University 420 White Building 10900 Euclid Avenue Cleveland, OH 44106-7221	Office Ph: 216 368-1366 Fax: 216 368-3209	175, 176, 177
Dr. Richard J. Matyi	Department of Materials Science & Engineering University of Wisconsin, Madison 1500 Engineering Drive Madison, WI 53706	Office Ph: 608 263-1716 Fax: 608 262-8353	897
Prof. Tony Maxworthy	Department of Aerospace Engineering OHE 430 University of Southern California 854 West 36th Place, RRB 101 Los Angeles, CA 90089-1191	Office Ph: 213 740-0481 Fax: 213 740-7774	899, 901

Prof. Mark J. McCready	Department of Chemical Engineering University of Notre Dame 182 Fitzpatrick Hall Notre Dame, IN 46556 Office Ph: 219 631-7146 Fax: 219 631-8366	600, 602
Dr. Paul J. McGinn	Department of Chemical Engineering University of Notre Dame 275 Fitzpatrick Hall Notre Dame, IN 46556 Office Ph: 219 631-6151 Fax: 219 631-8366	903
Prof. Gareth H. McKinley	Division of Applied Sciences Harvard University Pierce Hall, Room 316 Cambridge, MA 02138 Office Ph: 617 496-5167 Fax: 617 495-9837	104
Prof. J. T. McKinnon	Department of Chemical Engineering and Petroleum Refining Colorado School of Mines Golden, CO 80401 Office Ph: 303 273-3098 Fax: 303 273-3730	412
Dr. Alexander McPherson, Jr.	Department of Biochemistry Boyce Hall, Room 2466 University of California, Riverside 900 University Avenue Riverside, CA 92521-0129 Office Ph: 909 787-5391 Fax: 909 787-3790	19, 22
Dr. John McQuillen	Microgravity Fluids Branch Mail Stop 500-102 NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191 Office Ph: 216 433-2876 Fax: 216 433-8660	106
Prof. Eckart H. Meiburg	Department of Aerospace Engineering University of Southern California 846 West 36th Place, RRB 101 Los Angeles, CA 90089-1191 Office Ph: 213 740-5376 Fax: 213 740-7774	905
Prof. Suresh Menon	School of Aerospace Engineering Georgia Institute of Technology Atlanta, GA 30332-0150 Office Ph: 404 853-9160 Fax: 404 894-2760	414
Prof. Herman Merte, Jr.	Mechanical Engineering Department University of Michigan 2250 G. G. Brown Building Ann Arbor, MI 48109-2125 Office Ph: 313 764-5240 Fax: 313 747-3170	107, 603, 605

Prof. Horst Meyer	Department of Physics Duke University Durham, NC 27708-0305	
	Office Ph: 919 660-2520 Fax: 919 660-2521	755, 757
Mr. William V. Meyer	Ohio Aerospace Institute Mail Stop 105-1 NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191	
	Office Ph: 216 433-5011 Fax: 216 433-5033	1015
Dr. Fletcher J. Miller	Mail Stop 110-3 Case Western Reserve University NASA Lewis Research Center Cleveland, OH 44135-3191	
	Office Ph: 216 433-8845 Fax: 216 433-3793	416
Prof. John J. Moore	Department of Metallurgical and Materials Engineering Colorado School of Mines Golden, CO 80401	
	Office Ph: 303 273-3770 Fax: 303 273-3795	418, 907
Dr. D. J. Morré	Department of Medicinal Chemistry HANS 136 Purdue University South University Street West Lafayette, IN 47904	
	Office Ph: 317 494-1388 Fax: 317 494-4007	288
Prof. David W. Murhammer	Department of Chemical and Biochemical Engineering University of Iowa 125 B Chemistry Building Iowa City, IA 52242	
	Office Ph: 319 335-1228 Fax: 319 335-1415	291
Dr. Allan S. Myerson	Department of Chemical Engineering Polytechnic University Six Metrotech Center Brooklyn, NY 11201	
	Office Ph: 718 260-3223 Fax: 718 260-3776	909
Dr. Ali Nadim	College of Engineering Boston University 110 Cummington Street Boston, MA 02215	
	Office Ph: 617 353-3951 Fax: 617 353-5866	606

Prof. Warren Nagourney	Department of Physics College of Arts and Science Box 351560 University of Washington Seattle, WA 98195	Office Ph: 206 543-9585 Fax: 206 685-0635	759
Prof. Masami Nakagawa	Division of Engineering Colorado School of Mines 2425 Ridgcrest Drive, SE Golden, CO 80401-1887	Office Ph: 303 273-3524 Fax: 303 273-3602	608
Prof. Ranga Narayanan	Department of Chemical Engineering University of Florida 227 Chemical Engineering Building Gainesville, FL 32611	Office Ph: 352 392-9103 Fax: 352 392-9513	911
Dr. Vedha Nayagam	Analex Corporation 3001 Aerospace Parkway Brook Park, OH 44142	Office Ph: 216 433-8702 Fax: 216 433-8660	422
Prof. G. P. Neitzel	George W. Woodruff School of Mechanical Engineering Georgia Institute of Technology Atlanta, GA 30332-0405	Office Ph: 404 894-3242 Fax: 404 894-2291	610, 612
Prof. Kim O'Connor	Department of Chemical Engineering Tulane University Boggs Center, Suite 300 New Orleans, LA 70118	Office Ph: 504 865-5740 Fax: 504 865-6744	295
Dr. Hasan N. Oguz	Department of Mechanical Engineering Johns Hopkins University 3400 North Charles Street Baltimore, MD 21218-2686	Office Ph: 410 516-4651 Fax: 410 516-7254	613
Dr. Daniel R. Ohlsen	Program in Atmospheric and Oceanic Sciences Campus Box 311 University of Colorado, Boulder Boulder, CO 80309-0311	Office Ph: 303 492-8237 Fax: 303 492-3524	615
Prof. Simon Ostrach	Department of Mechanical & Aerospace Engineering 418 Glennan Building Case Western Reserve University 10900 Euclid Avenue Cleveland, OH 44106	Office Ph: 216 368-2942 Fax: 216 368-6445	109, 616, 618

Dr. Aleksandar G. Ostrogorsky	Department of Mechanical Engineering, Aeronautical Engineering, and Mechanics JEC 2026 Rensselaer Polytechnic Institute Troy, NY 12180-3590	Office Ph: 518 276-6975 Fax: 518 276-6025	179, 913
Dr. Ben Ovary	Mail Stop 110-3 Nyma, Inc. NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135	Office Ph: 216 433-8335 Fax: 216 433-3797	1018
Dr. Mark S. Paley	Space Sciences Laboratory Mail Code ES76 Universities Space Research Association NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812	Office Ph: 205 544-7775 Fax: 205 544-2102	915
Dr. Witold Palosz	Space Sciences Laboratory Mail Stop ES75 Universities Space Research Association NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812	Office Ph: 205 544-1272 Fax: 205 544-8762	917, 919
Dr. Bernhard O. Palsson	Department of Bioengineering Mail Code 0412 University of California, San Diego 9500 Gilman Drive La Jolla, , CA 92093-0412	Office Ph: 619 534-5668 Fax: 619 822-0240	298
Prof. Chang-Won Park	Department of Chemical Engineering University of Florida 227 Chemical Engineering Building Gainesville, FL 32611-2022	Office Ph: 352 392-6205 Fax: 352 392-9513	620
Prof. Alexander Z. Patashinski	Department of Physics and Astronomy Northwestern University 2145 Sheridan Road Evanston, IL 60208-3112	Office Ph: 847 467-2618 Fax: 847 491-9982	621, 760
Dr. Howard G. Pearlman	Mail Stop 500-115 NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191	Office Ph: 216 433-3710 Fax: 216 433-9419	58

Dr. David Pearson	Mail Stop 79-24 Jet Propulsion Laboratory (JPL) California Institute of Technology 4800 Oak Grove Drive Pasadena, CA 91109-8099	Office Ph: 818 394-9766 Fax: 818 393-4878	762
Dr. Neal R. Pellis	Biotechnology Program Mail Code SD3 NASA Johnson Space Center 2101 NASA Road One Houston, TX 77058	Office Ph: 713 483-2357 Fax: 713 483-3058	300
Prof. Jerome K. Percus	Courant Institute New York University 251 Mercer Street New York, NY 10012	Office Ph: 212 998-3130 Fax: 212 995-4121	623
Prof. John H. Perepezko	Department of Materials Science and Engineering University of Wisconsin, Madison 1509 University Avenue Madison, WI 53706-1595	Office Ph: 608 263-1678 Fax: 608 262-8353	920, 922, 924
Dr. Marc Perlin	Department of Naval Architecture & Marine Engineering College of Engineering University of Michigan 208 NAME Building Ann Arbor, MI 48109-2145	Office Ph: 313 763-4754 Fax: 313 763-3488	624
Prof. David R. Poirier	Department of Materials Science and Engineering College of Engineering & Mines University of Arizona Tucson, AZ 85721	Office Ph: 520 621-6072 Fax: 520 621-8059	181, 926
Dr. Dimos Poulikakos	Department of Mechanical Engineering University of Illinois, Chicago 842 West Taylor Street Chicago, IL 60607-7022	Office Ph: 312 996-3436 Fax: 312 413-0447	626
Prof. Andrea Prosperetti	Department of Mechanical Engineering Johns Hopkins University 122 Latrobe Hall Baltimore, MD 21218	Office Ph: 410 516-8534 Fax: 410 516-7254	627

Dr. Marc L. Pusey	Biophysics Branch Microgravity Science and Applications Division Mail Code ES76 NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812 Office Ph: 205 544-7823 Fax: 205 544-6660	302, 304, 1020
Dr. Seth J. Putterman	Department of Physics University of California, Los Angeles 405 Hilgard Avenue Los Angeles, CA 90024-1547 Office Ph: 310 825-2269 Fax: 310 206-5668	628
Dr. Peter J. Quesenberry	Cancer Center University of Massachusetts Medical Center Two Biotech 373 Plantation Street, Suite 202 Worcester, MA 01605 Office Ph: 508 856-6956 Fax: 508 856-1310	306
Prof. Dennis W. Readey	Coors Professor of Ceramic Engineering Department of Metallurgical and Materials Engineering Colorado School of Mines Golden, CO 80401 Office Ph: 303 273-3770 Fax: 303 273-3795	928
Dr. Liya L. Regel	International Center for Gravity Materials Science and Applications Clarkson University Box 5814 Potsdam, NY 13699-5814 Office Ph: 315 268-7672 Fax: 315 268-3833	932
Dr. Won-Kyu Rhim	Mechanical Systems Engineering and Research Division Mail Stop 183-401 Jet Propulsion Laboratory (JPL) California Institute of Technology 4800 Oak Grove Drive Pasadena, CA 91109-8099 Office Ph: 818 354-2925 Fax: 818 393-5039	934, 936
Dr. David C. Richardson	Department of Biochemistry Duke University Medical Center Box 3711 211 Nanaline Duke Building Durham, NC 27710 Office Ph: 919 684-6010 Fax: 919 684-8885	308
Dr. Michael B. Robinson	Crystal Growth and Solidification Branch Microgravity Science and Applications Division Mail Code ES75 NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812 Office Ph: 205 544-7774 Fax: 205 544-2176	938, 940, 941, 942

Dr. Chris B. Rogers	Department of Mechanical Engineering Tufts University Medford, MA 02155	Office Ph: 617 628-5000 Fax: 617 627-3819	629
Prof. Paul D. Ronney	Department of Mechanical Engineering OHE 430L University of Southern California University Park Los Angeles, CA 90089-1453	Office Ph: 213 740-0490 Fax: 213 740-8071	60, 423, 425, 631
Prof. Franz E. Rosenberger	Center for Microgravity and Materials Research University of Alabama, Huntsville Research Institute, Room M65 Huntsville, AL 35899	Office Ph: 205 890-6050 Fax: 205 890-6791	183, 185, 310, 313
Dr. Charles S. Rosenblatt	Department of Physics Case Western Reserve University Cleveland, OH 44106-7079	Office Ph: 216 368-4125 Fax: 216 368-4671	944
Prof. Daniel E. Rosner	Department of Chemical Engineering Mason Laboratory Yale University 9 Hillhouse Avenue, Room 319, P.O. Box 2159, Y.S. New Haven, CT 06520-8286	Office Ph: 203 432-4391 Fax: 203 432-7232	633, 635
Dr. Howard D. Ross	Mail Stop 500-115 NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191	Office Ph: 216 433-2562 Fax: 216 433-8660	63, 427
Dr. Joseph Rudnick	Department of Physics University of California, Los Angeles 405 Hilgard Avenue Los Angeles, CA 90024-1547	Office Ph: 310 825-8535 Fax: 310 476-4241	763
Dr. Gary A. Ruff	Department of Mechanical Engineering & Mechanics Drexel University 32nd and Chestnut Streets Philadelphia, PA 19104	Office Ph: 215 895-2352 Fax: 215 895-1478	430
Dr. Robert T. Ruggeri	The Boeing Company P.O. Box 3707 Seattle, WA 98124-2207	Office Ph: 206 773-8908 Fax: 206 773-2250	636

Dr. Albert Sacco	Department of Chemical Engineering Worcester Polytechnic Institute 100 Institute Road Worcester, MA 01609	Office Ph: 508 831-5333 Fax: 508 831-5853	946
Prof. Satwindar S. Sadhal	Department of Mechanical Engineering University of Southern California Los Angeles, CA 90089-1453	Office Ph: 213 740-0492 Fax: 213 740-0492	637, 640
Prof. W. M. Saltzman	School of Chemical Engineering Cornell University 120 Olin Hall Ithaca, NY 14853	Office Ph: 607 255-2657 Fax: 607 255-1136	316
Prof. Ashok S. Sangani	Department of Chemical Engineering & Material Science Syracuse University Syracuse, NY 13244-1190	Office Ph: 315 443-4502 Fax: 315 443-2559	112, 641
Prof. Robert L. Sani	Department of Chemical Engineering ECCH 1-43, Campus Box 424 University of Colorado, Boulder Engineering Center Boulder, CO 80309-0424	Office Ph: 303 492-5517 Fax: 303 492-4341	114
Dr. Dudley A. Saville	Department of Chemical Engineering School of Engineering and Applied Science Princeton University Engineering Quadrangle, A-215 Princeton, NJ 08540-5263	Office Ph: 609 258-4585 Fax: 609 258-0211	116, 643
Dr. Michael F. Schatz	School of Physics Georgia Institute of Technology Atlanta, GA 30332-0430	Office Ph: 404 894-5201 Fax: 404 894-9958	645
Dr. Leonard W. Schwartz	Department of Engineering Spencer Laboratory University of Delaware Newark, DE 19716	Office Ph: 302 831-6830 Fax: 302 831-3619	647
Prof. George M. Seidel	Department of Physics Brown University Providence, RI 02912	Office Ph: 401 863-2584 Fax: 401 863-2024	765

Dr. Eric S. Shaqfeh	Department of Chemical Engineering Stanford University 207 Stauffer III Stanford, CA 94305	Office Ph: 415 723-4906 Fax: 415 723-9780	648
Prof. Benjamin D. Shaw	Department of Mechanical, Aeronautical & Materials Engineering College of Engineering University of California, Davis Davis, CA 95616-5294	Office Ph: 916 752-4130 Fax: 916 752-4158	66, 432, 650
Prof. Frank G. Shi	School of Engineering ZotCode 2575 University of California at Irvine 916 Engineering Tower Irvine, CA 92697-2575	Office Ph: 714 824-5362 Fax: 714 824-2541	947
Dr. Peter Shirron	Mail Stop 713 NASA Goddard Space Flight Center Greenbelt Road Greenbelt, MD 20771-0001	Office Ph: 301 286-7327 Fax: 301 286-1702	1023
Dr. J. M. Shoemaker	Science and Technology Division Aerospace Design and Fabrication, Inc. 2001 Aerospace Parkway Brookpark, OH 44125	Office Ph: 216 977-1137	1025
Dr. Joel A. Silver	Southwest Sciences, Inc. 1570 Pacheco Street, Suite E-11 Santa Fe, NM 87501	Office Ph: 505 984-1322 Fax: 505 988-9230	434
Dr. Bhim S. Singh	Mail Stop 500-327 NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191	Office Ph: 216 433-5396 Fax: 216 433-8660	652
Dr. Jogender Singh	Applied Research Laboratory Pennsylvania State University P.O. Box 30 University Park, PA 16804-0030	Office Ph: 814 863-9898 Fax: 814 863-1183	948
Dr. N. B. Singh	Westinghouse Electric Corporation 1310 Beulah Road Pittsburgh, PA 15235	Office Ph: 412 256-1469 Fax: 412 256-1661	950, 953

Dr. Gregory T. Smedley	Mail Code 210-41 California Institute of Technology 1201 East California Boulevard Pasadena, CA 91125 Office Ph: 818 395-4130 Fax: 818 568-8743	655
Dr. Craig D. Smith	Center for Macromolecular Crystallography 79-THT, BHSB 233a University of Alabama, Birmingham 1918 University Boulevard Birmingham, AL 35294-0005 Office Ph: 205 934-7233 Fax: 205 934-0480	319
Prof. Marc K. Smith	George W. Woodruff School of Mechanical Engineering Georgia Institute of Technology Atlanta, GA 30332-0405 Office Ph: 404 894-3826 Fax: 404 894-2291	657, 659
Prof. Mitchell D. Smooke	Department of Mechanical Engineering Yale University P.O. Box 2159 - Yale Station New Haven, CT 06520-2159 Office Ph: 203 432-4344 Fax: 203 433-6678	435
Dr. Siavash H. Sohrab	Department of Mechanical Engineering Technological Institute Northwestern University Evanston, IL 60208 Office Ph: 847 491-3572	437
Dr. Ain A. Sonin	Department of Mechanical Engineering Massachusetts Institute of Technology Cambridge, MA 02139-4307 Office Ph: 617 253-2247 Fax: 617 258-5802	660
Prof. Frans A. Spaepen	Division of Applied Sciences Harvard University Pierce Hall 29 Oxford Street Cambridge, MA 02193 Office Ph: 617 495-3760 Fax: 617 495-9837	955, 958
Dr. Kathleen J. Stebe	Department of Chemical Engineering Johns Hopkins University 3400 North Charles Street Baltimore, MD 21218-2694 Office Ph: 410 516-7769 Fax: 410 516-5510	662
Prof. Paul H. Steen	School of Chemical Engineering Cornell University Olin Hall Ithaca, NY 14853-5301 Office Ph: 607 255-8656 Fax: 607 255-9166	663, 665

Dr. Doru M. Stefanescu	Department of Metallurgical and Materials Engineering Solidification Laboratory University of Alabama, Tuscaloosa 141 Bevell Building P.O. Box 870202 Tuscaloosa, AL 35487-0202	Office Ph: 205 348-1749 Fax: 205 348-8574	187, 961
Dr. F. M. Stewart	Department of Medicine University of Massachusetts Medical Center 55 Lake Avenue, North Worcester, MA 01655	Office Ph: 508 856-3903 Fax: 508 856-6715	321
Dr. Donald M. Strayer	Mail Stop 79-24 Jet Propulsion Laboratory (JPL) California Institute of Technology 4800 Oak Grove Drive Pasadena, CA 91109-8099	Office Ph: 818 354-1698 Fax: 818 393-4878	766, 768
Dr. Stein Sture	Department of Civil, Environmental, and Architectural Engineering University of Colorado, Boulder Engineering Center OT6-26 Campus Box 428 Boulder, CO 80309-0428	Office Ph: 303 492-7651 Fax: 303 492-7317	117
Dr. Ching-Hua Su	Crystal Growth and Solidification Branch Microgravity Science and Applications Division Mail Code ES75 NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812	Office Ph: 205 544-7776 Fax: 205 544-8762	189
Prof. R. S. Subramanian	Department of Chemical Engineering Clarkson University Box 5705 Potsdam, NY 13699-5705	Office Ph: 315 268-6648 Fax: 315 268-6654	119, 667
Prof. Harry L. Swinney	Department of Physics Center for Nonlinear Dynamics University of Texas, Austin Austin, TX 78712-1111	Office Ph: 512 471-4619 Fax: 512 471-1558	668, 670
Dr. Frank R. Szofran	Microgravity Science and Applications Division Mail Code ES71 NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812	Office Ph: 205 544-7777 Fax: 205 544-8762	963, 965

Prof. James S. Tien	Mechanical and Aerospace Engineering 415 Glennan Hall Case Western Reserve University 10900 Euclid Avenue Cleveland, OH 44106 Office Ph: 216 368-4581 Fax: 216 368-6445	68
Dr. Daniel R. Talham	Department of Chemistry University of Florida P.O. Box 117200 Gainesville, FL 32611-7200 Office Ph: 352 392-9016 Fax: 352 392-3255	967
Prof. Saleh Tanveer	Department of Mathematics 100 Mathematics Building Ohio State University 231 West 18th Avenue Columbus, OH 43210-1174 Office Ph: 614 292-5710 Fax: 614 292-1479	672, 674
Dr. John M. Tarbell	Department of Chemical Engineering Physiological Transport Studies Laboratory Pennsylvania State University 111 Fenske Laboratory University Park, PA 16802-4400 Office Ph: 814 863-4801 Fax: 814 865-7846	677
Dr. Robert L. Thompson	Mail Stop 500-102 NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191 Office Ph: 216 433-3321 Fax: 216 433-8660	679
Dr. David M. Tiede	Chemistry Division Argonne National Laboratory Building 200, Room E113 9700 South Cass Avenue Argonne, IL 60439 Office Ph: 630 252-3539 Fax: 630 252-9289	323
Dr. Paul Todd	Department of Chemical Engineering University of Colorado, Boulder Campus Box 424 Boulder, CO 80309-0424 Office Ph: 303 492-5936 Fax: 303 492-4341	325
Prof. Penger Tong	Department of Physics Oklahoma State University Stillwater, OK 74078-0266 Office Ph: 405 744-5800 Fax: 405 744-6811	680, 682

Prof. Jose L. Torero	Department of Fire Protection Engineering University of Maryland, College Park 0150 Engineering Classroom Building College Park, MD 20742-3031	Office Ph: 301 405-3992 Fax: 301 405-9383	439
Dr. John M. Torkelson	Department of Chemical Engineering Northwestern University Evanston, IL 60208-3120	Office Ph: 847 491-7449 Fax: 847 491-3728	969
Dr. Bruce Towe	Bioengineering Program College of Engineering and Applied Sciences Arizona State University Box 876006 Tempe, AZ 85287	Office Ph: 602 965-4116 Fax: 602 965-8013	328
Dr. Eugene H. Trinh	Mechanical Systems Engineering and Research Division Mail Stop 183-401 Jet Propulsion Laboratory (JPL) 4800 Oak Grove Drive Pasadena, CA 91109-8099	Office Ph: 818 354-7125 Fax: 818 393-5039	331, 684, 972
Dr. Rohit K. Trivedi	Department of Materials Science and Engineering Iowa State University Ames, IA 50011	Office Ph: 515 294-5869 Fax: 515 294-4291	191
Dr. James D. Trolinger	MetroLaser, Inc. 18006 Skypark Circle, #108 Irvine, CA 92614	Office Ph: 714 553-0688 Fax: 714 553-0495	974
Prof. Grétar Tryggvason	Department of Mechanical Engineering University of Michigan 2250 G. G. Brown Building Ann Arbor, MI 48109-2125	Office Ph: 313 763-1049 Fax: 313 764-4256	686, 976
Prof. John Tsamopoulos	Department of Chemical Engineering State University of New York, Buffalo 507 Furnas Hall Buffalo, NY 14260	Office Ph: 716 645-6229 Fax: 716 645-3822	688
Dr. David L. Urban	Mail Stop 500-115 NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191	Office Ph: 216 433-2835 Fax: 216 433-8660	441

Dr. Randall L. Vander Wal	Mail Stop 110-3 NASA Lewis Research Center 21000 Brookpark Road Cleveland, OH 44135-3191	Office Ph: 216 433-9065 Fax: 216 433-3793	1027
Prof. Arvind Varma	Department of Chemical Engineering University of Notre Dame Nortre Dame, IN 46556	Office Ph: 219 631-6491 Fax: 219 631-8366	443
Prof. Jorge Viñals	Supercomputer Computations Research Institute Mail Code B-186 Florida State University 444 Science Center Library Tallahassee, FL 32306-4032	Office Ph: 904 644-1010 Fax: 904 644-0098	691, 693
Dr. Viola Vogel	Center for Bioengineering University of Washington Box 357962 Seattle, WA 98195	Office Ph: 206 543-1776 Fax: 206 685-4434	333
Dr. Martin P. Volz	Crystal Growth and Solidification Branch Microgravity Science and Applications Division Mail Code ES75 NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812	Office Ph: 205 544-5078 Fax: 205 544-8762	978
Prof. Peter W. Voorhees	Department of Materials Science and Engineering Northwestern University 2145 Sheridan Road Evanston, IL 60208-3108	Office Ph: 847 491-3537 Fax: 847-491-7820	193
Dr. John S. Walker	Department of Mechanical and Industrial Engineering University of Illinois at Urbana 140 Mechanical Engineering Building 1206 West Green Street Urbana, IL 61801	Office Ph: 217 333-7979 Fax: 217 244-6534	980
Prof. Taylor G. Wang	Center for Microgravity Research & Applications Vanderbilt University Box 1743, Station B Nashville, TN 37240	Office Ph: 615 343-6965 Fax: 615 343-8730	121

Dr. Keith B. Ward	Laboratory for the Structure of Matter Mail Code 6030 Naval Research Laboratory (NRL) 4555 Overlook Avenue, SW Washington, DC 20375-5000	Office Ph: 202 767-2735 Fax: 202 767-6874	23, 336
Prof. Peter C. Wayner, Jr.	Isermann Department of Chemical Engineering Rensselaer Polytechnic Institute Troy, NY 12180	Office Ph: 518 276-6199 Fax: 518 276-4030	123, 695
Dr. Richard Weber	Containerless Research, Inc. 910 University Place Evanston, IL 60201-3149	Office Ph: 847 467-2678 Fax: 847 467-2679	982
Prof. David A. Weitz	Department of Physics and Astronomy University of Pennsylvania 209 South 33rd Street Philadelphia, PA 19104-6396	Office Ph: 215 898-7522 Fax: 215 898-2010	124
Prof. John S. Wettlaufer	Applied Physics Laboratory Box 355640 University of Washington Seattle, WA 98105	Office Ph: 206 543-7224 Fax: 206 543-3521	985
Prof. Indrek S. Wichman	Department of Mechanical Engineering Michigan State University East Lansing, MI 48824	Office Ph: 517 353-9180 Fax: 517 353-1750	445
Dr. Heribert Wiedemeier	Department of Chemistry 211 MRC Rensselaer Polytechnic Institute Troy, NY 12180-3590	Office Ph: 518 276-8444 Fax: 518 276-8554	195, 987
Dr. John M. Wiencek	Department of Chemical and Biochemical Engineering College of Engineering University of Iowa 125B Chemistry Building Iowa City, IA 52242	Office Ph: 319 353-2377 Fax: 319 335-1415	337
Dr. William R. Wilcox	International Center for Gravity, Materials Science, and Applications Clarkson University Potsdam, NY 13699-5814	Office Ph: 315 268-7672 Fax: 315 268-3833	988

Prof. Forman A. Williams	Department of Applied Mechanics University of California, San Diego Ames Hall, Department B-010 La Jolla, CA 92093-0411	
	Office Ph: 619 534-5492 Fax: 619 534-5354	71, 447
Dr. W. W. Wilson	Department of Chemistry Mississippi State University Box 9573 Mississippi State, MS 39762-5613	
	Office Ph: 601 325-3584 Fax: 601 325-1618	339, 341
Dr. Michael Winter	Mail Stop 90 United Technologies Research Center East Hartford, CT 06108	
	Office Ph: 203 727-7805 Fax: 203 727-7911	449
Dr. William K. Witherow	Biophysics Branch Microgravity Science and Applications Division Mail Code ES76 NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812	
	Office Ph: 205 544-7811 Fax: 205 544-2102	342
Dr. August F. Witt	Department of Materials Science & Engineering Massachusetts Institute of Technology Room 13-4134 77 Massachusetts Avenue Cambridge, MA 02139-4307	
	Office Ph: 617 253-5303 Fax: 617 253-5827	990
Prof. Larry Witte	Department of Mechanical Engineering University of Houston 4800 Calhoun Road Houston, TX 77204-4792	
	Office Ph: 713 743-4501 Fax: 713 743-4503	697
Prof. M. G. Worster	Department of Engineering Science and Applied Mathematics Northwestern University 633 Clark Street Evanston, IL 60201	
	Office Ph: 847 491-3345 Fax: 01223337918	699
Dr. Xiao-lun Wu	Department of Physics and Astronomy University of Pittsburgh Pittsburgh, PA 15260	
	Office Ph: 412 624-0873 Fax: 412 624-9163	701
Dr. Jiann C. Yang	Fire Sensing and Extinguishment Group Building and Fire Research Laboratory National Institute of Standards and Technology Gaithersburg, MD 20899	
	Office Ph: 301 975-6662 Fax: 301 975-4052	452

Prof. Abdelfattah Zebib	Department of Mechanical and Aerospace Engineering Rutgers University P.O. Box 909 Piscataway, NJ 08855-0909	
	Office Ph: 908 445-2248 Fax: 908 932-5313	704
Mr. Frank R. Zimmerman	Metallurgy Research and Development Branch Metallic Materials and Processes Division Mail Code EH23-S NASA Marshall Space Flight Center Marshall Space Flight Center, AL 35812	
	Office Ph: 205 544-4958 Fax: 205 544-0212	1030
Dr. Charles F. Zukoski	Department of Chemical Engineering University of Illinois at Urbana-Champaign 114 Roger Adams Laboratory 600 South Matthews Street Urbana, IL 61801	
	Office Ph: 217 333-5076 Fax: 217 244-8068	344

